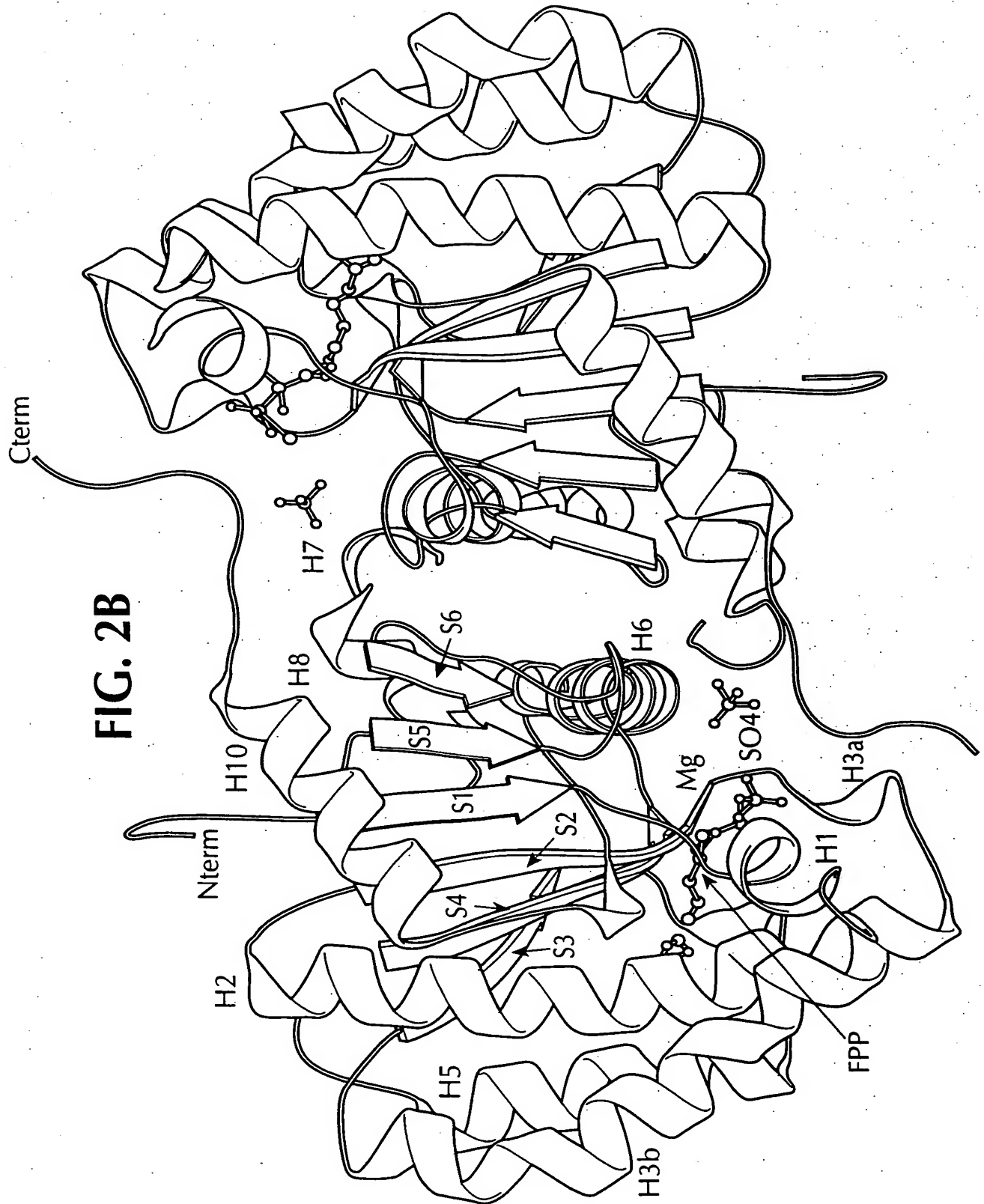
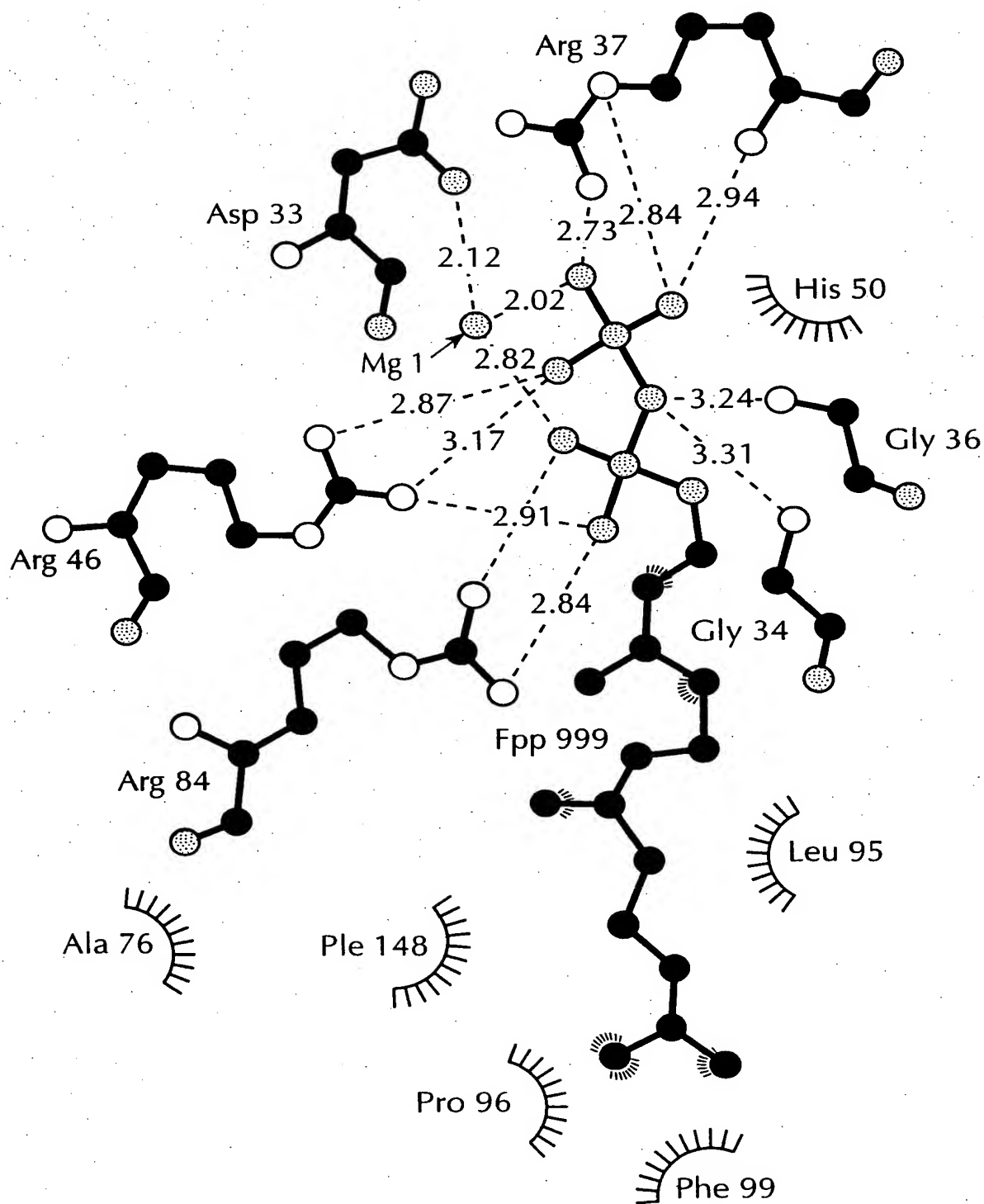


FIG. 2A



**FIG. 3**

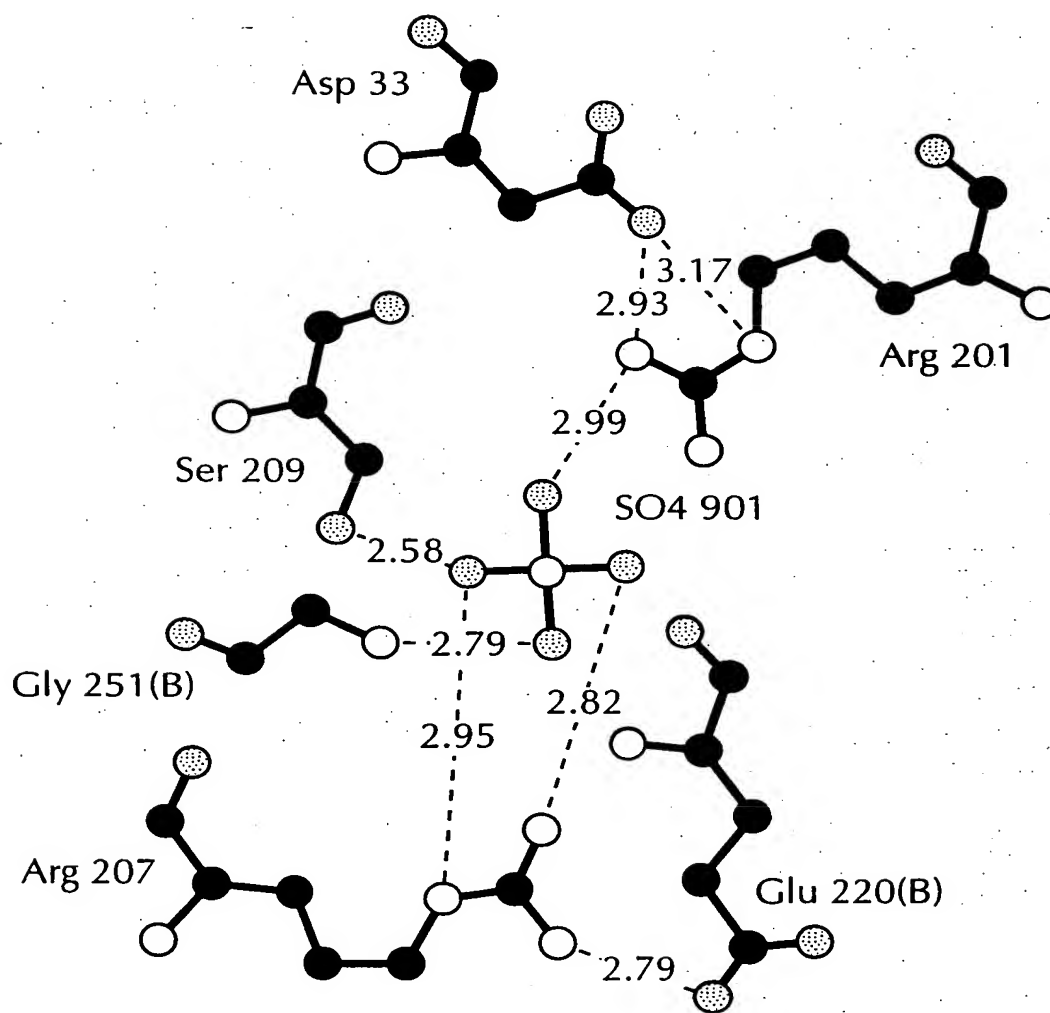
**FIG. 4**

Figure S-1

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REMARK This is upps_18.pdb. Final refined coordinates
REMARK Se-Met residues are labelled as MET.
REMARK The waters coordinating Mg have chain ID Y, and all others have id W
CRYST1 58.187 58.187 159.260 90.00 90.00 90.00 P 41 21 2
SCALE1 0.017186 0.000000 0.000000 0.000000
SCALE2 0.000000 0.017186 0.000000 0.000000
SCALE3 0.000000 0.000000 0.006279 0.000000
ATOM 1 N LEU A 19 35.033 -14.033 23.925 1.00 29.71 N
ATOM 3 CA LEU A 19 33.645 -13.527 23.662 1.00 28.44 C
ATOM 5 CB LEU A 19 33.433 -12.200 24.386 1.00 29.20 C
ATOM 8 CG LEU A 19 33.497 -12.174 25.905 1.00 30.93 C
ATOM 10 CD1 LEU A 19 33.365 -10.745 26.347 1.00 30.45 C
ATOM 14 CD2 LEU A 19 32.446 -13.079 26.546 1.00 32.94 C
ATOM 18 C LEU A 19 33.290 -13.243 22.196 1.00 28.33 C
ATOM 19 O LEU A 19 34.152 -12.853 21.381 1.00 28.39 O
ATOM 22 N ASP A 20 32.043 -13.522 21.852 1.00 26.28 N
ATOM 24 CA ASP A 20 31.430 -12.987 20.654 1.00 25.36 C
ATOM 26 CB ASP A 20 30.114 -13.715 20.440 1.00 25.86 C
ATOM 29 CG ASP A 20 29.338 -13.191 19.252 1.00 28.24 C
ATOM 30 OD1 ASP A 20 29.702 -12.116 18.720 1.00 27.94 O
ATOM 31 OD2 ASP A 20 28.346 -13.782 18.780 1.00 28.73 O
ATOM 32 C ASP A 20 31.284 -11.448 20.847 1.00 25.10 C
ATOM 33 O ASP A 20 30.422 -10.971 21.609 1.00 22.59 O
ATOM 34 N SER A 21 32.161 -10.687 20.182 1.00 24.38 N
ATOM 36 CA SER A 21 32.201 -9.250 20.334 1.00 25.01 C
ATOM 38 CB SER A 21 33.558 -8.635 19.892 1.00 24.93 C
ATOM 41 OG SER A 21 33.778 -8.777 18.504 1.00 30.57 O
ATOM 43 C SER A 21 31.009 -8.563 19.659 1.00 23.77 C
ATOM 44 O SER A 21 30.757 -7.411 19.943 1.00 23.66 O
ATOM 45 N SER A 22 30.264 -9.281 18.813 1.00 23.46 N
ATOM 47 CA SER A 22 29.006 -8.768 18.259 1.00 23.43 C
ATOM 49 CB SER A 22 28.644 -9.438 16.934 1.00 24.22 C
ATOM 52 OG SER A 22 28.122 -10.727 17.122 1.00 24.09 O
ATOM 54 C SER A 22 27.810 -8.939 19.191 1.00 22.93 C
ATOM 55 O SER A 22 26.694 -8.605 18.803 1.00 23.33 O
ATOM 56 N ASN A 23 28.007 -9.575 20.352 1.00 20.84 N
ATOM 58 CA ASN A 23 26.875 -9.820 21.302 1.00 19.62 C
ATOM 60 CB ASN A 23 26.384 -11.251 21.172 1.00 18.76 C
ATOM 63 CG ASN A 23 25.113 -11.536 21.976 1.00 21.31 C
ATOM 64 OD1 ASN A 23 24.298 -10.647 22.196 1.00 22.93 O
ATOM 65 ND2 ASN A 23 24.926 -12.813 22.369 1.00 17.10 N
ATOM 68 C ASN A 23 27.219 -9.495 22.777 1.00 19.72 C
ATOM 69 O ASN A 23 26.911 -10.255 23.717 1.00 20.19 O
ATOM 70 N ILE A 24 27.815 -8.351 22.950 1.00 20.07 N
ATOM 72 CA ILE A 24 28.017 -7.801 24.267 1.00 19.87 C
ATOM 74 CB ILE A 24 28.992 -6.710 24.240 1.00 20.02 C

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Figure S-2

ATOM	76	CG1	ILE	A	24	30.345	-7.120	23.579	1.00	19.94	C
ATOM	79	CD1	ILE	A	24	30.888	-8.399	24.046	1.00	24.18	C
ATOM	83	CG2	ILE	A	24	29.233	-6.194	25.663	1.00	18.86	C
ATOM	87	C	ILE	A	24	26.635	-7.338	24.764	1.00	19.12	C
ATOM	88	O	ILE	A	24	25.962	-6.552	24.107	1.00	19.21	O
ATOM	89	N	PRO	A	25	26.201	-7.824	25.916	1.00	19.24	N
ATOM	90	CA	PRO	A	25	24.934	-7.368	26.506	1.00	18.36	C
ATOM	92	CB	PRO	A	25	24.915	-7.997	27.889	1.00	18.96	C
ATOM	95	CG	PRO	A	25	26.102	-8.809	28.010	1.00	18.56	C
ATOM	98	CD	PRO	A	25	26.855	-8.857	26.735	1.00	19.05	C
ATOM	101	C	PRO	A	25	24.905	-5.887	26.693	1.00	17.44	C
ATOM	102	O	PRO	A	25	25.893	-5.268	27.089	1.00	15.46	O
ATOM	103	N	GLU	A	26	23.730	-5.303	26.481	1.00	15.44	N
ATOM	105	CA	GLU	A	26	23.637	-3.878	26.633	1.00	16.23	C
ATOM	107	CB	GLU	A	26	22.449	-3.320	25.840	1.00	17.12	C
ATOM	110	CG	GLU	A	26	22.548	-3.704	24.368	1.00	18.68	C
ATOM	113	CD	GLU	A	26	21.640	-2.901	23.452	1.00	21.85	C
ATOM	114	OE1	GLU	A	26	20.565	-2.505	23.896	1.00	18.93	O
ATOM	115	OE2	GLU	A	26	22.025	-2.645	22.276	1.00	23.48	O
ATOM	116	C	GLU	A	26	23.524	-3.482	28.105	1.00	16.17	C
ATOM	117	O	GLU	A	26	23.977	-2.411	28.512	1.00	16.61	O
ATOM	118	N	HIS	A	27	22.869	-4.317	28.894	1.00	15.09	N
ATOM	120	CA	HIS	A	27	22.602	-3.979	30.303	1.00	13.86	C
ATOM	122	CB	HIS	A	27	21.169	-3.471	30.454	1.00	14.52	C
ATOM	125	CG	HIS	A	27	20.807	-3.047	31.846	1.00	13.99	C
ATOM	126	ND1	HIS	A	27	19.547	-2.631	32.210	1.00	13.45	N
ATOM	128	CE1	HIS	A	27	19.544	-2.299	33.501	1.00	14.66	C
ATOM	130	NE2	HIS	A	27	20.759	-2.467	33.975	1.00	15.65	N
ATOM	132	CD2	HIS	A	27	21.572	-2.938	32.970	1.00	15.42	C
ATOM	134	C	HIS	A	27	22.842	-5.181	31.192	1.00	13.69	C
ATOM	135	O	HIS	A	27	22.174	-6.177	31.040	1.00	14.43	O
ATOM	136	N	ILE	A	28	23.813	-5.069	32.114	1.00	13.47	N
ATOM	138	CA	ILE	A	28	24.143	-6.115	33.106	1.00	12.14	C
ATOM	140	CB	ILE	A	28	25.633	-6.505	33.077	1.00	12.79	C
ATOM	142	CG1	ILE	A	28	26.033	-7.122	31.694	1.00	14.15	C
ATOM	145	CD1	ILE	A	28	27.552	-7.405	31.516	1.00	14.23	C
ATOM	149	CG2	ILE	A	28	25.909	-7.568	34.205	1.00	14.07	C
ATOM	153	C	ILE	A	28	23.800	-5.526	34.469	1.00	11.97	C
ATOM	154	O	ILE	A	28	24.102	-4.405	34.736	1.00	13.91	O
ATOM	155	N	ALA	A	29	23.090	-6.293	35.296	1.00	11.82	N
ATOM	157	CA	ALA	A	29	22.679	-5.872	36.585	1.00	12.85	C
ATOM	159	CB	ALA	A	29	21.121	-5.930	36.677	1.00	14.01	C
ATOM	163	C	ALA	A	29	23.276	-6.875	37.525	1.00	12.33	C
ATOM	164	O	ALA	A	29	23.216	-8.083	37.266	1.00	12.21	O
ATOM	165	N	ILE	A	30	23.910	-6.383	38.569	1.00	13.85	N
ATOM	167	CA	ILE	A	30	24.578	-7.242	39.519	1.00	12.99	C
ATOM	169	CB	ILE	A	30	26.105	-6.952	39.505	1.00	12.60	C
ATOM	171	CG1	ILE	A	30	26.682	-7.208	38.127	1.00	15.31	C

Figure 5-3

ATOM	174	CD1	ILE	A	30	28.108	-6.809	38.004	1.00	16.29	C
ATOM	178	CG2	ILE	A	30	26.806	-7.805	40.574	1.00	14.00	C
ATOM	182	C	ILE	A	30	24.150	-7.055	40.968	1.00	12.79	C
ATOM	183	O	ILE	A	30	24.159	-5.944	41.477	1.00	14.09	O
ATOM	184	N	ILE	A	31	23.847	-8.154	41.650	1.00	12.48	N
ATOM	186	CA	ILE	A	31	23.551	-8.105	43.081	1.00	13.09	C
ATOM	188	CB	ILE	A	31	22.553	-9.121	43.465	1.00	11.75	C
ATOM	190	CG1	ILE	A	31	21.174	-8.742	42.825	1.00	13.25	C
ATOM	193	CD1	ILE	A	31	20.156	-9.766	42.973	1.00	12.90	C
ATOM	197	CG2	ILE	A	31	22.335	-9.189	45.034	1.00	15.80	C
ATOM	201	C	ILE	A	31	24.889	-8.373	43.769	1.00	13.23	C
ATOM	202	O	ILE	A	31	25.392	-9.477	43.731	1.00	14.66	O
ATOM	203	N	MET	A	32	25.434	-7.351	44.376	1.00	15.78	N
ATOM	205	CA	MET	A	32	26.787	-7.426	44.960	1.00	16.24	C
ATOM	207	CB	MET	A	32	27.365	-6.045	45.157	1.00	16.42	C
ATOM	210	CG	MET	A	32	27.891	-5.340	43.828	1.00	17.63	C
ATOM	213	SE	MET	A	32	28.542	-3.613	44.076	1.00	22.61	SE
ATOM	214	CE	MET	A	32	27.255	-2.828	44.924	1.00	14.77	C
ATOM	218	C	MET	A	32	26.538	-8.142	46.288	1.00	17.32	C
ATOM	219	O	MET	A	32	25.757	-7.657	47.110	1.00	20.89	O
ATOM	220	N	ASP	A	33	27.079	-9.328	46.468	1.00	18.33	N
ATOM	222	CA	ASP	A	33	26.756	-10.082	47.678	1.00	16.55	C
ATOM	224	CB	ASP	A	33	25.602	-11.059	47.451	1.00	17.43	C
ATOM	227	CG	ASP	A	33	24.966	-11.557	48.753	1.00	17.30	C
ATOM	228	OD1	ASP	A	33	25.318	-10.996	49.855	1.00	13.13	O
ATOM	229	OD2	ASP	A	33	24.093	-12.463	48.739	1.00	15.77	O
ATOM	230	C	ASP	A	33	28.003	-10.812	48.146	1.00	17.89	C
ATOM	231	O	ASP	A	33	28.890	-11.168	47.322	1.00	15.75	O
ATOM	232	N	GLY	A	34	28.079	-11.034	49.470	1.00	17.72	N
ATOM	234	CA	GLY	A	34	29.241	-11.715	50.069	1.00	18.78	C
ATOM	237	C	GLY	A	34	30.348	-10.861	50.730	1.00	19.87	C
ATOM	238	O	GLY	A	34	31.387	-11.406	51.165	1.00	19.72	O
ATOM	239	N	ASN	A	35	30.162	-9.550	50.806	1.00	19.48	N
ATOM	241	CA	ASN	A	35	31.120	-8.703	51.500	1.00	18.76	C
ATOM	243	CB	ASN	A	35	30.683	-7.260	51.489	1.00	17.54	C
ATOM	246	CG	ASN	A	35	30.826	-6.585	50.103	1.00	17.11	C
ATOM	247	OD1	ASN	A	35	31.338	-7.186	49.132	1.00	19.59	O
ATOM	248	ND2	ASN	A	35	30.409	-5.328	50.022	1.00	18.12	N
ATOM	251	C	ASN	A	35	31.393	-9.135	52.967	1.00	19.03	C
ATOM	252	O	ASN	A	35	32.527	-9.182	53.370	1.00	18.97	O
ATOM	253	N	GLY	A	36	30.359	-9.376	53.773	1.00	20.74	N
ATOM	255	CA	GLY	A	36	30.567	-9.759	55.176	1.00	21.53	C
ATOM	258	C	GLY	A	36	31.201	-11.128	55.341	1.00	23.14	C
ATOM	259	O	GLY	A	36	32.102	-11.289	56.178	1.00	24.55	O
ATOM	260	N	ARG	A	37	30.761	-12.104	54.553	1.00	21.56	N
ATOM	262	CA	ARG	A	37	31.399	-13.431	54.528	1.00	21.24	C
ATOM	264	CB	ARG	A	37	30.685	-14.373	53.589	1.00	21.38	C

Figure S-4

ATOM	267	CG	ARG	A	37	29.551	-15.084	54.251	1.00	21.21	C
ATOM	270	CD	ARG	A	37	28.656	-15.797	53.253	1.00	23.93	C
ATOM	273	NE	ARG	A	37	27.859	-14.811	52.517	1.00	22.62	N
ATOM	275	CZ	ARG	A	37	26.980	-15.116	51.571	1.00	21.04	C
ATOM	276	NH1	ARG	A	37	26.822	-16.374	51.209	1.00	22.62	N
ATOM	279	NH2	ARG	A	37	26.262	-14.134	51.000	1.00	20.48	N
ATOM	282	C	ARG	A	37	32.902	-13.383	54.167	1.00	20.23	C
ATOM	283	O	ARG	A	37	33.725	-14.070	54.813	1.00	19.75	O
ATOM	284	N	TRP	A	38	33.260	-12.519	53.232	1.00	19.40	N
ATOM	286	CA	TRP	A	38	34.611	-12.336	52.826	1.00	20.13	C
ATOM	288	CB	TRP	A	38	34.653	-11.268	51.739	1.00	19.45	C
ATOM	291	CG	TRP	A	38	35.994	-11.109	51.144	1.00	20.31	C
ATOM	292	CD1	TRP	A	38	36.512	-11.754	50.074	1.00	17.50	C
ATOM	294	NE1	TRP	A	38	37.792	-11.311	49.828	1.00	20.60	N
ATOM	296	CE2	TRP	A	38	38.097	-10.342	50.747	1.00	20.37	C
ATOM	297	CD2	TRP	A	38	36.990	-10.187	51.577	1.00	19.63	C
ATOM	298	CE3	TRP	A	38	37.054	-9.252	52.613	1.00	22.63	C
ATOM	300	CZ3	TRP	A	38	38.204	-8.533	52.778	1.00	22.44	C
ATOM	302	CH2	TRP	A	38	39.271	-8.698	51.945	1.00	24.20	C
ATOM	304	CZ2	TRP	A	38	39.250	-9.597	50.910	1.00	24.03	C
ATOM	306	C	TRP	A	38	35.451	-11.862	54.018	1.00	20.75	C
ATOM	307	O	TRP	A	38	36.602	-12.292	54.194	1.00	22.81	O
ATOM	308	N	ALA	A	39	34.919	-10.910	54.755	1.00	21.08	N
ATOM	310	CA	ALA	A	39	35.655	-10.406	55.936	1.00	22.51	C
ATOM	312	CB	ALA	A	39	35.048	-9.206	56.470	1.00	21.11	C
ATOM	316	C	ALA	A	39	35.728	-11.489	57.050	1.00	24.22	C
ATOM	317	O	ALA	A	39	36.816	-11.692	57.653	1.00	23.31	O
ATOM	318	N	LYS	A	40	34.600	-12.167	57.278	1.00	26.01	N
ATOM	320	CA	LYS	A	40	34.472	-13.172	58.339	1.00	29.48	C
ATOM	322	CB	LYS	A	40	33.086	-13.780	58.461	1.00	30.95	C
ATOM	325	CG	LYS	A	40	32.738	-14.139	59.954	1.00	36.08	C
ATOM	328	CD	LYS	A	40	31.382	-14.838	60.169	1.00	39.32	C
ATOM	331	CE	LYS	A	40	30.948	-14.773	61.659	1.00	42.36	C
ATOM	334	NZ	LYS	A	40	29.432	-14.866	61.939	1.00	40.77	N
ATOM	338	C	LYS	A	40	35.442	-14.281	58.100	1.00	29.66	C
ATOM	339	O	LYS	A	40	36.127	-14.706	59.022	1.00	32.17	O
ATOM	340	N	LYS	A	41	35.624	-14.696	56.851	1.00	29.31	N
ATOM	342	CA	LYS	A	41	36.663	-15.690	56.504	1.00	30.03	C
ATOM	344	CB	LYS	A	41	36.810	-15.898	54.989	1.00	30.35	C
ATOM	347	CG	LYS	A	41	35.700	-16.716	54.378	1.00	34.59	C
ATOM	350	CD	LYS	A	41	35.955	-17.036	52.938	1.00	38.67	C
ATOM	353	CE	LYS	A	41	34.861	-17.947	52.405	1.00	43.28	C
ATOM	356	NZ	LYS	A	41	35.184	-18.413	51.037	1.00	46.88	N
ATOM	360	C	LYS	A	41	38.050	-15.256	56.983	1.00	29.67	C

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Figure 5-5

ATOM	361	O	LYS	A	41	38.969	-16.085	57.147	1.00	28.21	O
ATOM	362	N	ARG	A	42	38.243	-13.953	57.120	1.00	28.87	N
ATOM	364	CA	ARG	A	42	39.562	-13.436	57.466	1.00	28.18	C
ATOM	366	CB	ARG	A	42	39.961	-12.313	56.501	1.00	29.35	C
ATOM	369	CG	ARG	A	42	40.021	-12.721	55.048	1.00	28.81	C
ATOM	372	CD	ARG	A	42	40.021	-11.591	54.028	1.00	30.63	C
ATOM	375	NE	ARG	A	42	40.388	-12.096	52.717	1.00	29.41	N
ATOM	377	CZ	ARG	A	42	39.674	-12.941	51.956	1.00	29.02	C
ATOM	378	NH1	ARG	A	42	38.455	-13.375	52.304	1.00	27.34	N
ATOM	381	NH2	ARG	A	42	40.213	-13.354	50.812	1.00	32.07	N
ATOM	384	C	ARG	A	42	39.616	-12.930	58.899	1.00	26.88	C
ATOM	385	O	ARG	A	42	40.696	-12.382	59.308	1.00	27.41	O
ATOM	386	N	LYS	A	43	38.573	-13.244	59.658	1.00	26.24	N
ATOM	388	CA	LYS	A	43	38.339	-12.785	61.016	1.00	27.28	C
ATOM	390	CB	LYS	A	43	39.358	-13.430	61.986	1.00	27.88	C
ATOM	393	CG	LYS	A	43	39.291	-14.931	61.947	1.00	28.59	C
ATOM	396	CD	LYS	A	43	38.104	-15.442	62.640	1.00	33.35	C
ATOM	399	CE	LYS	A	43	38.276	-16.978	62.818	1.00	38.43	C
ATOM	402	NZ	LYS	A	43	37.417	-17.508	63.913	1.00	41.99	N
ATOM	406	C	LYS	A	43	38.339	-11.255	61.155	1.00	27.79	C
ATOM	407	O	LYS	A	43	38.579	-10.714	62.260	1.00	28.30	O
ATOM	408	N	MET	A	44	38.032	-10.557	60.051	1.00	25.78	N
ATOM	410	CA	MET	A	44	37.942	-9.116	60.066	1.00	24.14	C
ATOM	412	CB	MET	A	44	38.546	-8.522	58.802	1.00	24.94	C
ATOM	415	CG	MET	A	44	39.959	-8.825	58.625	1.00	25.24	C
ATOM	418	SE	MET	A	44	41.036	-7.933	59.950	1.00	30.88	SE
ATOM	419	CE	MET	A	44	41.028	-6.193	59.231	1.00	25.65	C
ATOM	423	C	MET	A	44	36.482	-8.695	60.224	1.00	23.07	C
ATOM	424	O	MET	A	44	35.539	-9.481	60.007	1.00	23.62	O
ATOM	425	N	PRO	A	45	36.260	-7.468	60.653	1.00	21.02	N
ATOM	426	CA	PRO	A	45	34.912	-6.954	60.800	1.00	20.17	C
ATOM	428	CB	PRO	A	45	35.125	-5.533	61.318	1.00	20.67	C
ATOM	431	CG	PRO	A	45	36.473	-5.515	61.829	1.00	20.27	C
ATOM	434	CD	PRO	A	45	37.267	-6.453	60.962	1.00	22.00	C
ATOM	437	C	PRO	A	45	34.197	-6.854	59.442	1.00	18.68	C
ATOM	438	O	PRO	A	45	34.781	-6.724	58.372	1.00	18.23	O
ATOM	439	N	ARG	A	46	32.889	-6.902	59.538	1.00	19.31	N
ATOM	441	CA	ARG	A	46	31.959	-6.830	58.381	1.00	20.60	C
ATOM	443	CB	ARG	A	46	30.508	-6.844	58.873	1.00	20.47	C
ATOM	446	CG	ARG	A	46	29.978	-8.248	59.297	1.00	19.15	C
ATOM	449	CD	ARG	A	46	28.516	-8.291	59.565	1.00	17.43	C
ATOM	452	NE	ARG	A	46	27.736	-7.846	58.379	1.00	18.75	N
ATOM	454	CZ	ARG	A	46	27.475	-8.589	57.300	1.00	20.20	C
ATOM	455	NH1	ARG	A	46	27.761	-9.864	57.264	1.00	18.60	N
ATOM	458	NH2	ARG	A	46	26.879	-8.043	56.261	1.00	18.87	N

Figure S-6

ATOM	461	C	ARG	A	46	32.251	-5.594	57.477	1.00	20.94	C
ATOM	462	O	ARG	A	46	32.392	-5.682	56.221	1.00	20.74	O
ATOM	463	N	ILE	A	47	32.445	-4.449	58.126	1.00	21.03	N
ATOM	465	CA	ILE	A	47	32.730	-3.218	57.399	1.00	21.24	C
ATOM	467	CB	ILE	A	47	32.773	-1.972	58.346	1.00	21.32	C
ATOM	469	CG1	ILE	A	47	33.840	-2.122	59.431	1.00	23.48	C
ATOM	472	CD1	ILE	A	47	34.146	-0.742	60.107	1.00	25.40	C
ATOM	476	CG2	ILE	A	47	31.414	-1.688	58.981	1.00	23.53	C
ATOM	480	C	ILE	A	47	33.995	-3.358	56.533	1.00	21.27	C
ATOM	481	O	ILE	A	47	34.105	-2.713	55.467	1.00	20.38	O
ATOM	482	N	LYS	A	48	34.964	-4.165	56.945	1.00	20.58	N
ATOM	484	CA	LYS	A	48	36.147	-4.350	56.101	1.00	20.25	C
ATOM	486	CB	LYS	A	48	37.159	-5.227	56.832	1.00	20.22	C
ATOM	489	CG	LYS	A	48	38.448	-5.482	56.101	1.00	23.83	C
ATOM	492	CD	LYS	A	48	39.194	-4.199	55.912	1.00	29.06	C
ATOM	495	CE	LYS	A	48	40.587	-4.417	55.480	1.00	33.23	C
ATOM	498	NZ	LYS	A	48	41.293	-3.094	55.609	1.00	33.67	N
ATOM	502	C	LYS	A	48	35.831	-5.000	54.712	1.00	19.15	C
ATOM	503	O	LYS	A	48	36.498	-4.708	53.699	1.00	19.86	O
ATOM	504	N	GLY	A	49	34.844	-5.883	54.683	1.00	20.05	N
ATOM	506	CA	GLY	A	49	34.400	-6.508	53.447	1.00	17.92	C
ATOM	509	C	GLY	A	49	33.745	-5.437	52.559	1.00	18.99	C
ATOM	510	O	GLY	A	49	33.893	-5.429	51.326	1.00	19.22	O
ATOM	511	N	HIS	A	50	32.957	-4.581	53.173	1.00	18.74	N
ATOM	513	CA	HIS	A	50	32.342	-3.461	52.438	1.00	19.52	C
ATOM	515	CB	HIS	A	50	31.375	-2.735	53.311	1.00	17.59	C
ATOM	518	CG	HIS	A	50	30.163	-3.527	53.641	1.00	19.24	C
ATOM	519	ND1	HIS	A	50	29.521	-4.346	52.737	1.00	17.54	N
ATOM	521	CE1	HIS	A	50	28.463	-4.883	53.323	1.00	19.19	C
ATOM	523	NE2	HIS	A	50	28.407	-4.455	54.574	1.00	18.01	N
ATOM	525	CD2	HIS	A	50	29.442	-3.591	54.786	1.00	20.18	C
ATOM	527	C	HIS	A	50	33.378	-2.508	51.829	1.00	19.62	C
ATOM	528	O	HIS	A	50	33.227	-2.031	50.701	1.00	18.48	O
ATOM	529	N	TYR	A	51	34.431	-2.199	52.583	1.00	20.02	N
ATOM	531	CA	TYR	A	51	35.546	-1.463	52.052	1.00	21.38	C
ATOM	533	CB	TYR	A	51	36.641	-1.240	53.138	1.00	23.20	C
ATOM	536	CG	TYR	A	51	37.748	-0.373	52.626	1.00	25.21	C
ATOM	537	CD1	TYR	A	51	38.788	-0.918	51.880	1.00	31.67	C
ATOM	539	CE1	TYR	A	51	39.775	-0.128	51.362	1.00	31.55	C
ATOM	541	CZ	TYR	A	51	39.712	1.239	51.537	1.00	32.74	C
ATOM	542	OH	TYR	A	51	40.725	2.015	50.992	1.00	36.21	O
ATOM	544	CE2	TYR	A	51	38.679	1.808	52.225	1.00	32.92	C
ATOM	546	CD2	TYR	A	51	37.685	1.005	52.761	1.00	29.03	C
ATOM	548	C	TYR	A	51	36.123	-2.105	50.806	1.00	21.19	C
ATOM	549	O	TYR	A	51	36.290	-1.461	49.769	1.00	21.07	O

Figure S-8

ATOM	640	CD1	ILE	A	57	30.657	-0.576	44.434	1.00	21.39	C
ATOM	644	CG2	ILE	A	57	31.647	0.392	41.790	1.00	24.07	C
ATOM	648	C	ILE	A	57	34.008	-0.997	40.789	1.00	20.46	C
ATOM	649	O	ILE	A	57	33.617	-0.969	39.626	1.00	18.90	C
ATOM	650	N	LYS	A	58	35.211	-0.547	41.152	1.00	20.57	O
ATOM	652	CA	LYS	A	58	36.168	0.040	40.197	1.00	21.49	N
ATOM	654	CB	LYS	A	58	37.441	0.472	40.947	1.00	21.75	C
ATOM	657	CG	LYS	A	58	37.117	1.600	41.976	1.00	23.68	C
ATOM	660	CD	LYS	A	58	38.339	2.301	42.572	1.00	25.10	C
ATOM	663	CE	LYS	A	58	37.945	3.352	43.642	1.00	28.89	C
ATOM	666	NZ	LYS	A	58	38.859	3.440	44.858	1.00	24.42	N
ATOM	670	C	LYS	A	58	36.536	-0.938	39.117	1.00	22.38	C
ATOM	671	O	LYS	A	58	36.540	-0.646	37.898	1.00	22.61	N
ATOM	672	N	LYS	A	59	36.877	-2.121	39.575	1.00	21.83	O
ATOM	674	CA	LYS	A	59	37.333	-3.148	38.662	1.00	23.13	N
ATOM	676	CB	LYS	A	59	37.627	-4.438	39.403	1.00	22.24	C
ATOM	679	CG	LYS	A	59	38.792	-4.388	40.335	1.00	28.15	C
ATOM	682	CD	LYS	A	59	39.145	-5.776	40.848	1.00	31.71	C
ATOM	685	CE	LYS	A	59	40.139	-5.681	41.980	1.00	35.46	C
ATOM	688	NZ	LYS	A	59	40.432	-7.014	42.552	1.00	37.22	N
ATOM	692	C	LYS	A	59	36.267	-3.428	37.625	1.00	22.01	C
ATOM	693	O	LYS	A	59	36.534	-3.497	36.415	1.00	21.76	N
ATOM	694	N	ILE	A	60	35.050	-3.629	38.104	1.00	21.61	O
ATOM	696	CA	ILE	A	60	33.959	-4.029	37.208	1.00	20.73	N
ATOM	698	CB	ILE	A	60	32.793	-4.620	38.018	1.00	21.57	C
ATOM	700	CG1	ILE	A	60	33.300	-5.832	38.827	1.00	20.71	C
ATOM	703	CD1	ILE	A	60	34.249	-6.785	38.080	1.00	24.83	C
ATOM	707	CG2	ILE	A	60	31.725	-5.049	37.120	1.00	21.49	C
ATOM	711	C	ILE	A	60	33.527	-2.894	36.281	1.00	20.03	C
ATOM	712	O	ILE	A	60	33.157	-3.145	35.115	1.00	18.76	O
ATOM	713	N	THR	A	61	33.571	-1.664	36.784	1.00	19.70	N
ATOM	715	CA	THR	A	61	33.256	-0.497	35.991	1.00	20.75	C
ATOM	717	CB	THR	A	61	33.356	0.745	36.848	1.00	20.28	C
ATOM	719	OG1	THR	A	61	32.313	0.769	37.860	1.00	19.69	O
ATOM	721	CG2	THR	A	61	33.106	1.994	36.015	1.00	22.45	C
ATOM	725	C	THR	A	61	34.225	-0.419	34.808	1.00	20.83	C
ATOM	726	O	THR	A	61	33.845	-0.162	33.684	1.00	20.38	O
ATOM	727	N	ARG	A	62	35.500	-0.649	35.070	1.00	20.89	N
ATOM	729	CA	ARG	A	62	36.503	-0.580	34.014	1.00	20.61	C
ATOM	731	CB	ARG	A	62	37.900	-0.840	34.604	1.00	21.79	C
ATOM	734	CG	ARG	A	62	38.464	0.409	35.169	1.00	25.29	C
ATOM	737	CD	ARG	A	62	39.855	0.255	35.875	1.00	29.18	C
ATOM	740	NE	ARG	A	62	39.762	0.999	37.100	1.00	31.20	N
ATOM	742	CZ	ARG	A	62	40.565	0.906	38.119	1.00	38.16	C

Figure 5-9

ATOM	743	NH1	ARG	A	62	41.652	0.143	38.052	1.00	33.80	N
ATOM	746	NH2	ARG	A	62	40.281	1.604	39.216	1.00	39.36	N
ATOM	749	C	ARG	A	62	36.282	-1.572	32.914	1.00	20.18	C
ATOM	750	O	ARG	A	62	36.313	-1.205	31.711	1.00	21.54	O
ATOM	751	N	VAL	A	63	36.058	-2.817	33.294	1.00	17.83	N
ATOM	753	CA	VAL	A	63	35.911	-3.830	32.267	1.00	19.70	C
ATOM	755	CB	VAL	A	63	36.031	-5.289	32.804	1.00	20.08	C
ATOM	757	CG1	VAL	A	63	34.965	-5.592	33.788	1.00	24.62	C
ATOM	761	CG2	VAL	A	63	35.909	-6.270	31.685	1.00	21.24	C
ATOM	765	C	VAL	A	63	34.616	-3.598	31.507	1.00	18.94	C
ATOM	766	O	VAL	A	63	34.566	-3.781	30.281	1.00	19.67	O
ATOM	767	N	ALA	A	64	33.553	-3.229	32.210	1.00	19.11	N
ATOM	769	CA	ALA	A	64	32.294	-3.026	31.502	1.00	19.32	C
ATOM	771	CB	ALA	A	64	31.181	-2.696	32.458	1.00	18.08	C
ATOM	775	C	ALA	A	64	32.448	-1.887	30.453	1.00	19.80	C
ATOM	776	O	ALA	A	64	31.932	-1.998	29.348	1.00	19.72	O
ATOM	777	N	SER	A	65	33.136	-0.816	30.833	1.00	20.25	N
ATOM	779	CA	SER	A	65	33.369	0.299	29.929	1.00	21.02	C
ATOM	781	CB	SER	A	65	34.088	1.405	30.655	1.00	20.94	C
ATOM	784	OG	SER	A	65	34.286	2.541	29.848	1.00	21.89	O
ATOM	786	C	SER	A	65	34.231	-0.160	28.752	1.00	21.35	C
ATOM	787	O	SER	A	65	33.920	0.063	27.577	1.00	21.20	O
ATOM	788	N	ASP	A	66	35.325	-0.815	29.089	1.00	21.52	N
ATOM	790	CA	ASP	A	66	36.262	-1.292	28.091	1.00	22.65	C
ATOM	792	CB	ASP	A	66	37.432	-2.033	28.726	1.00	24.20	C
ATOM	795	CG	ASP	A	66	38.407	-1.104	29.403	1.00	25.17	C
ATOM	796	OD1	ASP	A	66	38.253	0.130	29.302	1.00	21.56	O
ATOM	797	OD2	ASP	A	66	39.356	-1.543	30.069	1.00	31.49	O
ATOM	798	C	ASP	A	66	35.626	-2.158	27.052	1.00	23.04	C
ATOM	799	O	ASP	A	66	36.025	-2.063	25.880	1.00	22.96	O
ATOM	800	N	ILE	A	67	34.668	-3.009	27.450	1.00	21.79	N
ATOM	802	CA	ILE	A	67	34.039	-3.932	26.503	1.00	21.75	C
ATOM	804	CB	ILE	A	67	33.806	-5.344	27.057	1.00	21.66	C
ATOM	806	CG1	ILE	A	67	32.605	-5.380	28.014	1.00	20.81	C
ATOM	809	CD1	ILE	A	67	32.303	-6.726	28.495	1.00	22.15	C
ATOM	813	CG2	ILE	A	67	35.045	-5.818	27.689	1.00	25.43	C
ATOM	817	C	ILE	A	67	32.768	-3.394	25.870	1.00	21.24	C
ATOM	818	O	ILE	A	67	32.251	-4.030	24.983	1.00	22.40	O
ATOM	819	N	GLY	A	68	32.316	-2.220	26.269	1.00	21.62	N
ATOM	821	CA	GLY	A	68	31.168	-1.620	25.602	1.00	20.70	C
ATOM	824	C	GLY	A	68	29.812	-2.051	26.108	1.00	20.05	C
ATOM	825	O	GLY	A	68	28.831	-2.057	25.365	1.00	19.84	O
ATOM	826	N	VAL	A	69	29.747	-2.414	27.385	1.00	19.04	N
ATOM	828	CA	VAL	A	69	28.448	-2.578	28.050	1.00	18.11	C
ATOM	830	CB	VAL	A	69	28.654	-3.171	29.472	1.00	17.55	C

[illegible]

Figure S-11

ATOM	927	CD1	LEU	A	74	28.559	-1.265	40.658	1.00	17.37	C
ATOM	931	CD2	LEU	A	74	27.273	-3.143	39.743	1.00	19.75	C
ATOM	935	C	LEU	A	74	23.852	-2.140	42.104	1.00	16.01	C
ATOM	936	O	LEU	A	74	23.494	-1.022	42.471	1.00	15.64	O
ATOM	937	N	TYR	A	75	23.457	-3.249	42.736	1.00	14.70	N
ATOM	939	CA	TYR	A	75	22.548	-3.202	43.883	1.00	16.58	C
ATOM	941	CB	TYR	A	75	21.901	-4.551	44.152	1.00	15.63	C
ATOM	944	CG	TYR	A	75	20.576	-4.623	44.937	1.00	16.83	C
ATOM	945	CD1	TYR	A	75	19.831	-3.502	45.300	1.00	18.35	C
ATOM	947	CE1	TYR	A	75	18.603	-3.631	45.966	1.00	21.86	C
ATOM	949	CZ	TYR	A	75	18.117	-4.871	46.249	1.00	19.55	C
ATOM	950	OH	TYR	A	75	16.909	-5.126	46.888	1.00	21.64	O
ATOM	952	CE2	TYR	A	75	18.835	-5.976	45.894	1.00	18.56	C
ATOM	954	CD2	TYR	A	75	20.064	-5.859	45.274	1.00	18.57	C
ATOM	956	C	TYR	A	75	23.408	-2.865	45.094	1.00	18.35	C
ATOM	957	O	TYR	A	75	24.081	-3.774	45.598	1.00	21.45	O
ATOM	958	N	ALA	A	76	23.349	-1.626	45.568	1.00	17.47	N
ATOM	960	CA	ALA	A	76	24.237	-1.160	46.630	1.00	17.29	C
ATOM	962	CB	ALA	A	76	24.783	0.207	46.319	1.00	17.97	C
ATOM	966	C	ALA	A	76	23.597	-1.180	48.002	1.00	17.82	C
ATOM	967	O	ALA	A	76	24.307	-1.474	48.975	1.00	17.78	O
ATOM	968	N	PHE	A	77	22.269	-0.965	48.089	1.00	14.95	N
ATOM	970	CA	PHE	A	77	21.591	-0.962	49.386	1.00	16.76	C
ATOM	972	CB	PHE	A	77	21.999	0.288	50.180	1.00	16.07	C
ATOM	975	CG	PHE	A	77	21.581	0.273	51.593	1.00	18.45	C
ATOM	976	CD1	PHE	A	77	20.294	0.627	51.953	1.00	17.72	C
ATOM	978	CE1	PHE	A	77	19.886	0.627	53.271	1.00	19.47	C
ATOM	980	CZ	PHE	A	77	20.751	0.246	54.243	1.00	19.89	C
ATOM	982	CE2	PHE	A	77	22.064	-0.111	53.912	1.00	18.12	C
ATOM	984	CD2	PHE	A	77	22.483	-0.077	52.585	1.00	19.62	C
ATOM	986	C	PHE	A	77	20.100	-1.034	49.128	1.00	16.03	C
ATOM	987	O	PHE	A	77	19.526	-0.190	48.427	1.00	17.01	O
ATOM	988	N	SER	A	78	19.442	-2.035	49.690	1.00	18.21	N
ATOM	990	CA	SER	A	78	18.009	-2.216	49.400	1.00	17.11	C
ATOM	992	CB	SER	A	78	17.671	-3.697	49.392	1.00	19.17	C
ATOM	995	OG	SER	A	78	17.498	-4.134	50.718	1.00	21.44	O
ATOM	997	C	SER	A	78	17.122	-1.576	50.446	1.00	18.07	C
ATOM	998	O	SER	A	78	17.583	-1.198	51.498	1.00	17.28	O
ATOM	999	N	THR	A	79	15.842	-1.453	50.137	1.00	18.20	N
ATOM	1001	CA	THR	A	79	14.891	-0.959	51.135	1.00	18.68	C
ATOM	1003	CB	THR	A	79	13.508	-0.777	50.515	1.00	19.32	C
ATOM	1005	OG1	THR	A	79	13.198	-1.906	49.667	1.00	19.77	O
ATOM	1007	CG2	THR	A	79	13.484	0.458	49.606	1.00	20.90	C
ATOM	1011	C	THR	A	79	14.831	-1.868	52.370	1.00	18.45	C
ATOM	1012	O	THR	A	79	14.411	-1.422	53.413	1.00	20.07	O

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Figure S-12

ATOM	1013	N	GLU	A	80	15.232	-3.132	52.297	1.00	16.77	N
ATOM	1015	CA	GLU	A	80	15.239	-4.004	53.474	1.00	17.60	C
ATOM	1017	CB	GLU	A	80	14.888	-5.505	53.105	1.00	15.95	C
ATOM	1020	CG	GLU	A	80	13.447	-5.739	52.619	1.00	18.53	C
ATOM	1023	CD	GLU	A	80	13.143	-5.022	51.308	1.00	16.51	C
ATOM	1024	OE1	GLU	A	80	13.816	-5.370	50.301	1.00	17.78	O
ATOM	1025	OE2	GLU	A	80	12.355	-4.034	51.296	1.00	17.75	O
ATOM	1026	C	GLU	A	80	16.559	-3.985	54.290	1.00	17.37	C
ATOM	1027	O	GLU	A	80	16.619	-4.569	55.413	1.00	17.97	O
ATOM	1028	N	ASN	A	81	17.617	-3.381	53.762	1.00	17.67	N
ATOM	1030	CA	ASN	A	81	18.936	-3.371	54.443	1.00	17.55	C
ATOM	1032	CB	ASN	A	81	20.103	-3.062	53.509	1.00	17.73	C
ATOM	1035	CG	ASN	A	81	20.401	-4.194	52.456	1.00	16.56	C
ATOM	1036	OD1	ASN	A	81	20.814	-3.888	51.393	1.00	16.65	O
ATOM	1037	ND2	ASN	A	81	20.196	-5.477	52.795	1.00	14.21	N
ATOM	1040	C	ASN	A	81	19.031	-2.428	55.653	1.00	19.21	C
ATOM	1041	O	ASN	A	81	20.013	-2.492	56.404	1.00	19.28	O
ATOM	1042	N	TRP	A	82	18.037	-1.570	55.826	1.00	20.09	N
ATOM	1044	CA	TRP	A	82	17.942	-0.713	56.998	1.00	21.65	C
ATOM	1046	CB	TRP	A	82	16.757	0.247	56.847	1.00	22.61	C
ATOM	1049	CG	TRP	A	82	16.872	1.234	55.712	1.00	23.06	C
ATOM	1050	CD1	TRP	A	82	16.205	1.205	54.539	1.00	22.96	C
ATOM	1052	NE1	TRP	A	82	16.567	2.278	53.758	1.00	24.72	N
ATOM	1054	CE2	TRP	A	82	17.483	3.022	54.438	1.00	26.44	C
ATOM	1055	CD2	TRP	A	82	17.703	2.388	55.666	1.00	23.78	C
ATOM	1056	CE3	TRP	A	82	18.613	2.973	56.554	1.00	24.76	C
ATOM	1058	CZ3	TRP	A	82	19.252	4.128	56.177	1.00	24.12	C
ATOM	1060	CH2	TRP	A	82	19.024	4.709	54.964	1.00	25.54	C
ATOM	1062	CZ2	TRP	A	82	18.142	4.191	54.077	1.00	25.51	C
ATOM	1064	C	TRP	A	82	17.762	-1.539	58.274	1.00	23.03	C
ATOM	1065	O	TRP	A	82	17.963	-1.030	59.347	1.00	24.27	O
ATOM	1066	N	SER	A	83	17.349	-2.798	58.179	1.00	24.22	N
ATOM	1068	CA	SER	A	83	17.230	-3.623	59.385	1.00	25.70	C
ATOM	1070	CB	SER	A	83	16.395	-4.868	59.078	1.00	27.16	C
ATOM	1073	OG	SER	A	83	17.102	-5.692	58.158	1.00	28.89	O
ATOM	1075	C	SER	A	83	18.606	-4.036	59.972	1.00	24.61	C
ATOM	1076	O	SER	A	83	18.648	-4.658	61.059	1.00	25.58	O
ATOM	1077	N	ARG	A	84	19.681	-3.728	59.262	1.00	22.35	N
ATOM	1079	CA	ARG	A	84	21.026	-4.101	59.705	1.00	21.32	C
ATOM	1081	CB	ARG	A	84	22.041	-4.102	58.537	1.00	20.99	C
ATOM	1084	CG	ARG	A	84	21.844	-5.244	57.526	1.00	19.61	C
ATOM	1087	CD	ARG	A	84	22.802	-5.157	56.378	1.00	18.70	C
ATOM	1090	NE	ARG	A	84	22.552	-6.241	55.414	1.00	19.86	N
ATOM	1092	CZ	ARG	A	84	23.442	-6.673	54.550	1.00	17.63	C

Figure S-13

ATOM	1093	NH1	ARG	A	84	24.667	-6.196	54.556	1.00	18.00	N
ATOM	1096	NH2	ARG	A	84	23.147	-7.648	53.692	1.00	20.96	N
ATOM	1099	C	ARG	A	84	21.522	-3.153	60.807	1.00	21.21	C
ATOM	1100	O	ARG	A	84	20.951	-2.086	61.003	1.00	20.73	O
ATOM	1101	N	PRO	A	85	22.550	-3.546	61.538	1.00	22.18	N
ATOM	1102	CA	PRO	A	85	23.034	-2.685	62.619	1.00	22.16	C
ATOM	1104	CB	PRO	A	85	24.250	-3.446	63.130	1.00	23.56	C
ATOM	1107	CG	PRO	A	85	23.972	-4.882	62.831	1.00	22.89	C
ATOM	1110	CD	PRO	A	85	23.377	-4.752	61.418	1.00	22.00	C
ATOM	1113	C	PRO	A	85	23.441	-1.288	62.153	1.00	22.39	C
ATOM	1114	O	PRO	A	85	24.030	-1.060	61.143	1.00	20.13	O
ATOM	1115	N	GLU	A	86	23.187	-0.324	63.005	1.00	24.30	N
ATOM	1117	CA	GLU	A	86	23.511	1.067	62.699	1.00	23.98	C
ATOM	1119	CB	GLU	A	86	23.334	1.857	63.976	1.00	24.00	C
ATOM	1122	CG	GLU	A	86	23.624	3.342	63.893	1.00	29.54	C
ATOM	1125	CD	GLU	A	86	23.584	3.937	65.297	1.00	32.02	C
ATOM	1126	OE1	GLU	A	86	24.590	3.778	66.079	1.00	29.40	O
ATOM	1127	OE2	GLU	A	86	22.490	4.437	65.628	1.00	34.55	O
ATOM	1128	C	GLU	A	86	24.920	1.291	62.153	1.00	23.58	C
ATOM	1129	O	GLU	A	86	25.090	1.961	61.141	1.00	23.88	O
ATOM	1130	N	SER	A	87	25.937	0.775	62.829	1.00	23.07	N
ATOM	1132	CA	SER	A	87	27.306	0.949	62.389	1.00	22.78	C
ATOM	1134	CB	SER	A	87	28.274	0.237	63.350	1.00	23.67	C
ATOM	1137	OG	SER	A	87	28.068	-1.146	63.296	1.00	23.70	O
ATOM	1139	C	SER	A	87	27.566	0.511	60.933	1.00	22.94	C
ATOM	1140	O	SER	A	87	28.359	1.122	60.223	1.00	22.02	O
ATOM	1141	N	GLU	A	88	26.941	-0.588	60.520	1.00	22.60	N
ATOM	1143	CA	GLU	A	88	27.121	-1.091	59.147	1.00	22.11	C
ATOM	1145	CB	GLU	A	88	26.623	-2.542	58.996	1.00	21.88	C
ATOM	1148	CG	GLU	A	88	26.869	-3.147	57.605	1.00	21.65	C
ATOM	1151	CD	GLU	A	88	26.532	-4.625	57.520	1.00	25.86	C
ATOM	1152	OE1	GLU	A	88	26.358	-5.247	58.585	1.00	24.26	O
ATOM	1153	OE2	GLU	A	88	26.471	-5.205	56.388	1.00	19.30	O
ATOM	1154	C	GLU	A	88	26.372	-0.186	58.165	1.00	22.26	C
ATOM	1155	O	GLU	A	88	26.919	0.140	57.114	1.00	21.18	O
ATOM	1156	N	VAL	A	89	25.162	0.230	58.515	1.00	21.07	N
ATOM	1158	CA	VAL	A	89	24.408	1.161	57.694	1.00	23.74	C
ATOM	1160	CB	VAL	A	89	23.058	1.403	58.334	1.00	23.03	C
ATOM	1162	CG1	VAL	A	89	22.206	2.384	57.526	1.00	24.51	C
ATOM	1166	CG2	VAL	A	89	22.261	0.087	58.457	1.00	22.42	C
ATOM	1170	C	VAL	A	89	25.152	2.499	57.546	1.00	24.83	C
ATOM	1171	O	VAL	A	89	25.322	3.007	56.448	1.00	24.78	O
ATOM	1172	N	ASN	A	90	25.687	3.007	58.660	1.00	26.25	N
ATOM	1174	CA	ASN	A	90	26.350	4.291	58.636	1.00	26.99	C
ATOM	1176	CB	ASN	A	90	26.797	4.740	60.022	1.00	27.71	C

Figure 5-14

ATOM	1179	CG	ASN	A	90	25.676	5.263	60.867	1.00	30.18	C
ATOM	1180	OD1	ASN	A	90	24.614	5.663	60.356	1.00	33.31	O
ATOM	1181	ND2	ASN	A	90	25.904	5.306	62.183	1.00	27.81	N
ATOM	1184	C	ASN	A	90	27.536	4.110	57.758	1.00	26.87	C
ATOM	1185	O	ASN	A	90	27.855	4.975	56.959	1.00	25.31	O
ATOM	1186	N	TYR	A	91	28.271	3.009	57.956	1.00	26.49	N
ATOM	1188	CA	TYR	A	91	29.434	2.730	57.146	1.00	26.11	C
ATOM	1190	CB	TYR	A	91	30.234	1.493	57.657	1.00	25.85	C
ATOM	1193	CG	TYR	A	91	31.620	1.359	57.048	1.00	23.96	C
ATOM	1194	CD1	TYR	A	91	32.716	2.048	57.590	1.00	26.70	C
ATOM	1196	CE1	TYR	A	91	34.001	1.932	57.046	1.00	24.19	C
ATOM	1198	CZ	TYR	A	91	34.218	1.117	56.002	1.00	22.80	C
ATOM	1199	OH	TYR	A	91	35.500	1.022	55.497	1.00	23.89	O
ATOM	1201	CE2	TYR	A	91	33.155	0.402	55.428	1.00	22.32	C
ATOM	1203	CD2	TYR	A	91	31.869	0.504	56.002	1.00	22.45	C
ATOM	1205	C	TYR	A	91	29.194	2.629	55.637	1.00	26.38	C
ATOM	1206	O	TYR	A	91	29.934	3.189	54.870	1.00	26.36	O
ATOM	1207	N	ILE	A	92	28.228	1.824	55.238	1.00	25.66	N
ATOM	1209	CA	ILE	A	92	27.926	1.673	53.827	1.00	26.12	C
ATOM	1211	CB	ILE	A	92	26.759	0.695	53.647	1.00	25.25	C
ATOM	1213	CG1	ILE	A	92	27.172	-0.739	54.034	1.00	25.39	C
ATOM	1216	CD1	ILE	A	92	26.034	-1.733	54.271	1.00	27.13	C
ATOM	1220	CG2	ILE	A	92	26.323	0.755	52.151	1.00	24.60	C
ATOM	1224	C	ILE	A	92	27.565	3.032	53.214	1.00	27.59	C
ATOM	1225	O	ILE	A	92	28.082	3.406	52.132	1.00	28.45	O
ATOM	1226	N	MET	A	93	26.732	3.760	53.931	1.00	30.11	N
ATOM	1228	CA	MET	A	93	26.186	5.045	53.468	1.00	31.68	C
ATOM	1230	CB	MET	A	93	25.097	5.529	54.407	1.00	31.81	C
ATOM	1233	CG	MET	A	93	23.843	4.723	54.373	1.00	33.79	C
ATOM	1236	SE	MET	A	93	22.946	5.208	52.683	1.00	37.35	SE
ATOM	1237	CE	MET	A	93	21.512	3.775	52.713	1.00	37.93	C
ATOM	1241	C	MET	A	93	27.268	6.103	53.334	1.00	33.11	C
ATOM	1242	O	MET	A	93	27.130	7.058	52.563	1.00	31.09	O
ATOM	1243	N	ASN	A	94	28.370	5.939	54.063	1.00	34.42	N
ATOM	1245	CA	ASN	A	94	29.420	6.920	53.971	1.00	35.78	C
ATOM	1247	CB	ASN	A	94	30.018	7.168	55.342	1.00	36.88	C
ATOM	1250	CG	ASN	A	94	29.940	8.622	55.706	1.00	40.75	C
ATOM	1251	OD1	ASN	A	94	28.899	9.097	56.232	1.00	44.24	O
ATOM	1252	ND2	ASN	A	94	30.994	9.371	55.360	1.00	39.41	N
ATOM	1255	C	ASN	A	94	30.473	6.588	52.930	1.00	35.56	C
ATOM	1256	O	ASN	A	94	31.221	7.471	52.511	1.00	36.62	O
ATOM	1257	N	LEU	A	95	30.462	5.354	52.428	1.00	35.16	N
ATOM	1259	CA	LEU	A	95	31.441	4.919	51.451	1.00	35.20	C
ATOM	1261	CB	LEU	A	95	31.307	3.426	51.164	1.00	35.67	C

Figure S-15

ATOM	1264	CG	LEU	A	95	31.880	2.412	52.174	1.00	35.50	C
ATOM	1266	CD1	LEU	A	95	31.653	0.979	51.681	1.00	36.67	C
ATOM	1270	CD2	LEU	A	95	33.372	2.628	52.370	1.00	37.30	C
ATOM	1274	C	LEU	A	95	31.449	5.687	50.111	1.00	35.38	C
ATOM	1275	O	LEU	A	95	32.501	5.823	49.492	1.00	33.83	O
ATOM	1276	N	PRO	A	96	30.296	6.125	49.616	1.00	34.73	N
ATOM	1277	CA	PRO	A	96	30.272	6.799	48.314	1.00	35.25	C
ATOM	1279	CB	PRO	A	96	28.799	7.177	48.139	1.00	34.92	C
ATOM	1282	CG	PRO	A	96	28.068	6.178	48.960	1.00	34.51	C
ATOM	1285	CD	PRO	A	96	28.950	5.973	50.180	1.00	35.30	C
ATOM	1288	C	PRO	A	96	31.169	8.019	48.233	1.00	36.21	C
ATOM	1289	O	PRO	A	96	31.757	8.235	47.167	1.00	36.04	O
ATOM	1290	N	VAL	A	97	31.255	8.788	49.308	1.00	36.88	N
ATOM	1292	CA	VAL	A	97	32.101	9.980	49.350	1.00	38.78	C
ATOM	1294	CB	VAL	A	97	32.215	10.503	50.772	1.00	38.85	C
ATOM	1296	CG1	VAL	A	97	32.949	11.806	50.794	1.00	41.28	C
ATOM	1300	CG2	VAL	A	97	30.821	10.670	51.450	1.00	39.81	C
ATOM	1304	C	VAL	A	97	33.509	9.648	48.838	1.00	39.33	C
ATOM	1305	O	VAL	A	97	34.075	10.300	47.956	1.00	40.53	O
ATOM	1306	N	ASN	A	98	34.030	8.539	49.307	1.00	39.52	N
ATOM	1308	CA	ASN	A	98	35.391	8.178	49.015	1.00	39.90	C
ATOM	1310	CB	ASN	A	98	35.870	7.452	50.247	1.00	40.81	C
ATOM	1313	CG	ASN	A	98	35.556	8.273	51.475	1.00	44.06	C
ATOM	1314	OD1	ASN	A	98	36.192	9.333	51.681	1.00	49.41	O
ATOM	1315	ND2	ASN	A	98	34.485	7.886	52.226	1.00	43.40	N
ATOM	1318	C	ASN	A	98	35.582	7.403	47.764	1.00	38.44	C
ATOM	1319	O	ASN	A	98	36.620	7.523	47.099	1.00	38.84	O
ATOM	1320	N	PHE	A	99	34.580	6.623	47.428	1.00	36.20	N
ATOM	1322	CA	PHE	A	99	34.615	5.957	46.175	1.00	35.85	C
ATOM	1324	CB	PHE	A	99	33.336	5.128	45.990	1.00	35.17	C
ATOM	1327	CG	PHE	A	99	33.178	4.571	44.616	1.00	35.66	C
ATOM	1328	CD1	PHE	A	99	33.846	3.419	44.250	1.00	34.98	C
ATOM	1330	CE1	PHE	A	99	33.730	2.904	43.010	1.00	35.99	C
ATOM	1332	CZ	PHE	A	99	32.918	3.526	42.078	1.00	38.11	C
ATOM	1334	CE2	PHE	A	99	32.222	4.681	42.424	1.00	36.09	C
ATOM	1336	CD2	PHE	A	99	32.360	5.194	43.696	1.00	37.89	C
ATOM	1338	C	PHE	A	99	34.709	7.136	45.160	1.00	34.75	C
ATOM	1339	O	PHE	A	99	35.593	7.179	44.313	1.00	34.21	O
ATOM	1340	N	LEU	A	100	33.828	8.113	45.310	1.00	35.01	N
ATOM	1342	CA	LEU	A	100	33.738	9.201	44.320	1.00	35.68	C
ATOM	1344	CB	LEU	A	100	32.422	9.959	44.476	1.00	35.41	C
ATOM	1347	CG	LEU	A	100	31.179	9.074	44.274	1.00	35.54	C
ATOM	1349	CD1	LEU	A	100	29.890	9.879	44.385	1.00	37.75	C
ATOM	1353	CD2	LEU	A	100	31.228	8.346	42.916	1.00	37.40	C
ATOM	1357	C	LEU	A	100	34.964	10.121	44.294	1.00	36.47	C

Figure S-16

ATOM	1358	O	LEU	A	100	35.505	10.414	43.239	1.00	35.38	O
ATOM	1359	N	LYS	A	101	35.422	10.566	45.453	1.00	38.08	N
ATOM	1361	CA	LYS	A	101	36.613	11.385	45.505	1.00	39.49	C
ATOM	1363	CB	LYS	A	101	36.953	11.725	46.965	1.00	41.05	C
ATOM	1366	CG	LYS	A	101	38.052	12.792	47.144	1.00	46.37	C
ATOM	1369	CD	LYS	A	101	38.519	12.864	48.609	1.00	52.03	C
ATOM	1372	CE	LYS	A	101	39.692	13.872	48.803	1.00	55.75	C
ATOM	1375	NZ	LYS	A	101	40.146	13.948	50.243	1.00	58.06	N
ATOM	1379	C	LYS	A	101	37.805	10.732	44.765	1.00	38.27	C
ATOM	1380	O	LYS	A	101	38.451	11.388	43.953	1.00	39.84	O
ATOM	1381	N	THR	A	102	38.092	9.455	44.941	1.00	36.74	N
ATOM	1383	CA	THR	A	102	39.264	8.915	44.254	1.00	36.55	C
ATOM	1385	CB	THR	A	102	39.823	7.648	44.929	1.00	36.57	C
ATOM	1387	OG1	THR	A	102	38.801	6.616	45.033	1.00	36.64	O
ATOM	1389	CG2	THR	A	102	40.258	7.939	46.358	1.00	38.30	C
ATOM	1393	C	THR	A	102	39.004	8.553	42.809	1.00	35.68	C
ATOM	1394	O	THR	A	102	39.934	8.514	41.998	1.00	36.33	O
ATOM	1395	N	PHE	A	103	37.745	8.300	42.483	1.00	34.11	N
ATOM	1397	CA	PHE	A	103	37.454	7.664	41.214	1.00	33.19	C
ATOM	1399	CB	PHE	A	103	36.614	6.414	41.480	1.00	34.10	C
ATOM	1402	CG	PHE	A	103	36.671	5.382	40.390	1.00	34.47	C
ATOM	1403	CD1	PHE	A	103	37.854	4.826	39.992	1.00	36.53	C
ATOM	1405	CE1	PHE	A	103	37.872	3.863	39.008	1.00	40.08	C
ATOM	1407	CZ	PHE	A	103	36.678	3.450	38.446	1.00	38.01	C
ATOM	1409	CE2	PHE	A	103	35.516	4.007	38.885	1.00	37.20	C
ATOM	1411	CD2	PHE	A	103	35.528	4.952	39.827	1.00	36.15	C
ATOM	1413	C	PHE	A	103	36.775	8.603	40.216	1.00	31.94	C
ATOM	1414	O	PHE	A	103	36.721	8.266	39.051	1.00	31.23	O
ATOM	1415	N	LEU	A	104	36.406	9.788	40.673	1.00	31.41	N
ATOM	1417	CA	LEU	A	104	35.717	10.795	39.830	1.00	31.88	C
ATOM	1419	CB	LEU	A	104	35.388	12.069	40.600	1.00	32.95	C
ATOM	1422	CG	LEU	A	104	33.911	12.495	40.531	1.00	35.86	C
ATOM	1424	CD1	LEU	A	104	33.784	13.934	40.903	1.00	36.79	C
ATOM	1428	CD2	LEU	A	104	33.241	12.231	39.177	1.00	36.09	C
ATOM	1432	C	LEU	A	104	36.534	11.128	38.590	1.00	30.87	C
ATOM	1433	O	LEU	A	104	36.023	11.056	37.450	1.00	28.96	O
ATOM	1434	N	PRO	A	105	37.806	11.477	38.770	1.00	29.71	N
ATOM	1435	CA	PRO	A	105	38.665	11.720	37.613	1.00	28.88	C
ATOM	1437	CB	PRO	A	105	40.059	11.946	38.257	1.00	29.75	C
ATOM	1440	CG	PRO	A	105	39.769	12.486	39.568	1.00	29.64	C
ATOM	1443	CD	PRO	A	105	38.540	11.700	40.031	1.00	30.70	C
ATOM	1446	C	PRO	A	105	38.673	10.573	36.597	1.00	27.43	C
ATOM	1447	O	PRO	A	105	38.556	10.861	35.417	1.00	28.39	O
ATOM	1448	N	GLU	A	106	38.747	9.305	37.001	1.00	25.67	N
ATOM	1450	CA	GLU	A	106	38.785	8.205	36.013	1.00	26.46	C

Figure 5-17

ATOM	1452	CB	GLU A 106	39.266	6.879	36.672	1.00	25.85	C
ATOM	1455	CG	GLU A 106	39.073	5.636	35.844	1.00	30.43	C
ATOM	1458	CD	GLU A 106	39.977	4.441	36.192	1.00	34.88	C
ATOM	1459	OE1	GLU A 106	40.864	4.496	37.074	1.00	36.21	O
ATOM	1460	OE2	GLU A 106	39.825	3.406	35.511	1.00	40.24	O
ATOM	1461	C	GLU A 106	37.404	8.032	35.324	1.00	24.80	C
ATOM	1462	O	GLU A 106	37.334	7.772	34.127	1.00	24.07	O
ATOM	1463	N	LEU A 107	36.334	8.145	36.096	1.00	24.94	N
ATOM	1465	CA	LEU A 107	34.948	8.088	35.524	1.00	24.81	C
ATOM	1467	CB	LEU A 107	33.924	8.368	36.621	1.00	24.88	C
ATOM	1470	CG	LEU A 107	33.811	7.256	37.699	1.00	26.06	C
ATOM	1472	CD1	LEU A 107	32.865	7.552	38.865	1.00	26.08	C
ATOM	1476	CD2	LEU A 107	33.324	6.004	36.961	1.00	29.26	C
ATOM	1480	C	LEU A 107	34.816	9.131	34.399	1.00	25.29	C
ATOM	1481	O	LEU A 107	34.265	8.873	33.353	1.00	23.92	O
ATOM	1482	N	ILE A 108	35.325	10.312	34.667	1.00	26.19	N
ATOM	1484	CA	ILE A 108	35.282	11.404	33.730	1.00	26.70	C
ATOM	1486	CB	ILE A 108	35.719	12.695	34.378	1.00	26.11	C
ATOM	1488	CG1	ILE A 108	34.633	13.218	35.308	1.00	28.10	C
ATOM	1491	CD1	ILE A 108	35.006	14.376	36.181	1.00	26.75	C
ATOM	1495	CG2	ILE A 108	36.100	13.729	33.269	1.00	28.26	C
ATOM	1499	C	ILE A 108	36.150	11.095	32.532	1.00	27.93	C
ATOM	1500	O	ILE A 108	35.690	11.244	31.419	1.00	28.01	O
ATOM	1501	N	GLU A 109	37.358	10.592	32.755	1.00	28.79	N
ATOM	1503	CA	GLU A 109	38.247	10.227	31.684	1.00	29.48	C
ATOM	1505	CB	GLU A 109	39.625	9.847	32.280	1.00	31.35	C
ATOM	1508	CG	GLU A 109	40.759	9.600	31.279	1.00	35.99	C
ATOM	1511	CD	GLU A 109	42.077	9.229	31.976	1.00	42.41	C
ATOM	1512	OE1	GLU A 109	42.341	9.728	33.101	1.00	47.32	O
ATOM	1513	OE2	GLU A 109	42.856	8.425	31.432	1.00	49.04	O
ATOM	1514	C	GLU A 109	37.683	9.067	30.845	1.00	28.39	C
ATOM	1515	O	GLU A 109	37.868	9.028	29.639	1.00	27.13	O
ATOM	1516	N	LYS A 110	36.970	8.143	31.485	1.00	25.35	N
ATOM	1518	CA	LYS A 110	36.445	6.977	30.798	1.00	26.04	C
ATOM	1520	CB	LYS A 110	36.351	5.790	31.761	1.00	26.97	C
ATOM	1523	CG	LYS A 110	37.677	5.124	32.092	1.00	31.06	C
ATOM	1526	CD	LYS A 110	37.448	3.631	32.465	1.00	33.34	C
ATOM	1529	CE	LYS A 110	38.595	2.769	32.003	1.00	38.02	C
ATOM	1532	NZ	LYS A 110	39.912	3.292	32.530	1.00	39.14	N
ATOM	1536	C	LYS A 110	35.043	7.271	30.159	1.00	24.90	C
ATOM	1537	O	LYS A 110	34.414	6.392	29.595	1.00	23.07	O
ATOM	1538	N	ASN A 111	34.612	8.517	30.262	1.00	24.73	N
ATOM	1540	CA	ASN A 111	33.367	8.996	29.640	1.00	24.74	C
ATOM	1542	CB	ASN A 111	33.472	8.888	28.117	1.00	24.86	C
ATOM	1545	CG	ASN A 111	32.262	9.517	27.366	1.00	25.57	C
ATOM	1546	OD1	ASN A 111	31.633	10.456	27.839	1.00	25.66	O

Figure 5-18

ATOM	1547	ND2	ASN	A	111	31.953	8.968	26.199	1.00	25.94	N
ATOM	1550	C	ASN	A	111	32.165	8.237	30.215	1.00	23.43	C
ATOM	1551	O	ASN	A	111	31.228	7.935	29.486	1.00	22.32	O
ATOM	1552	N	VAL	A	112	32.245	7.941	31.531	1.00	21.22	N
ATOM	1554	CA	VAL	A	112	31.195	7.221	32.277	1.00	20.83	C
ATOM	1556	CB	VAL	A	112	31.790	6.302	33.409	1.00	19.69	C
ATOM	1558	CG1	VAL	A	112	30.593	5.613	34.195	1.00	20.14	C
ATOM	1562	CG2	VAL	A	112	32.618	5.310	32.836	1.00	20.50	C
ATOM	1566	C	VAL	A	112	30.203	8.150	32.894	1.00	19.35	C
ATOM	1567	O	VAL	A	112	30.596	9.174	33.480	1.00	21.72	O
ATOM	1568	N	LYS	A	113	28.908	7.835	32.785	1.00	20.43	N
ATOM	1570	CA	LYS	A	113	27.844	8.644	33.370	1.00	20.49	C
ATOM	1572	CB	LYS	A	113	26.687	8.861	32.369	1.00	21.50	C
ATOM	1575	CG	LYS	A	113	25.545	9.746	32.924	1.00	24.08	C
ATOM	1578	CD	LYS	A	113	24.558	10.228	31.790	1.00	28.15	C
ATOM	1581	CE	LYS	A	113	23.215	10.866	32.266	1.00	31.60	C
ATOM	1584	NZ	LYS	A	113	23.092	11.381	33.621	1.00	36.00	N
ATOM	1588	C	LYS	A	113	27.264	8.011	34.634	1.00	19.51	C
ATOM	1589	O	LYS	A	113	26.729	6.918	34.556	1.00	21.27	O
ATOM	1590	N	VAL	A	114	27.360	8.688	35.760	1.00	19.08	N
ATOM	1592	CA	VAL	A	114	26.836	8.183	37.028	1.00	19.56	C
ATOM	1594	CB	VAL	A	114	27.580	8.731	38.199	1.00	19.00	C
ATOM	1596	CG1	VAL	A	114	27.034	8.140	39.512	1.00	19.03	C
ATOM	1600	CG2	VAL	A	114	29.072	8.471	38.104	1.00	21.17	C
ATOM	1604	C	VAL	A	114	25.358	8.538	37.218	1.00	19.64	C
ATOM	1605	O	VAL	A	114	24.946	9.714	37.075	1.00	21.35	O
ATOM	1606	N	GLU	A	115	24.562	7.519	37.487	1.00	19.24	N
ATOM	1608	CA	GLU	A	115	23.143	7.650	37.770	1.00	18.63	C
ATOM	1610	CB	GLU	A	115	22.320	7.133	36.585	1.00	18.96	C
ATOM	1613	CG	GLU	A	115	22.648	7.917	35.313	1.00	20.87	C
ATOM	1616	CD	GLU	A	115	21.571	7.899	34.226	1.00	27.57	C
ATOM	1617	OE1	GLU	A	115	20.424	7.503	34.481	1.00	28.24	O
ATOM	1618	OE2	GLU	A	115	21.896	8.323	33.108	1.00	30.43	O
ATOM	1619	C	GLU	A	115	22.798	6.843	39.006	1.00	18.89	C
ATOM	1620	O	GLU	A	115	23.650	6.123	39.504	1.00	18.94	O
ATOM	1621	N	THR	A	116	21.575	7.018	39.503	1.00	17.89	N
ATOM	1623	CA	THR	A	116	21.042	6.265	40.627	1.00	18.76	C
ATOM	1625	CB	THR	A	116	21.094	7.014	42.014	1.00	18.92	C
ATOM	1627	OG1	THR	A	116	20.419	8.282	41.973	1.00	20.77	O
ATOM	1629	CG2	THR	A	116	22.530	7.318	42.462	1.00	19.10	C
ATOM	1633	C	THR	A	116	19.602	5.923	40.377	1.00	20.22	C
ATOM	1634	O	THR	A	116	18.879	6.652	39.653	1.00	20.69	O
ATOM	1635	N	ILE	A	117	19.202	4.820	41.010	1.00	19.42	N
ATOM	1637	CA	ILE	A	117	17.796	4.496	41.189	1.00	18.29	C

Figure 5-19

ATOM	1639	CB	ILE	A	117	17.318	3.284	40.379	1.00	17.89	C
ATOM	1641	CG1	ILE	A	117	18.143	2.046	40.710	1.00	16.30	C
ATOM	1644	CD1	ILE	A	117	17.717	0.887	39.886	1.00	14.98	C
ATOM	1648	CG2	ILE	A	117	17.357	3.572	38.896	1.00	18.08	C
ATOM	1652	C	ILE	A	117	17.602	4.252	42.686	1.00	17.90	C
ATOM	1653	O	ILE	A	117	18.495	3.723	43.382	1.00	18.47	O
ATOM	1654	N	GLY	A	118	16.437	4.579	43.197	1.00	18.03	N
ATOM	1656	CA	GLY	A	118	16.167	4.403	44.593	1.00	19.83	C
ATOM	1659	C	GLY	A	118	15.691	5.702	45.193	1.00	21.68	C
ATOM	1660	O	GLY	A	118	15.591	6.686	44.459	1.00	22.78	O
ATOM	1661	N	PHE	A	119	15.359	5.666	46.463	1.00	24.23	N
ATOM	1663	CA	PHE	A	119	14.853	6.829	47.183	1.00	27.03	C
ATOM	1665	CB	PHE	A	119	13.773	6.403	48.152	1.00	26.81	C
ATOM	1668	CG	PHE	A	119	12.702	5.628	47.485	1.00	26.22	C
ATOM	1669	CD1	PHE	A	119	12.766	4.248	47.454	1.00	28.52	C
ATOM	1671	CE1	PHE	A	119	11.783	3.512	46.846	1.00	27.75	C
ATOM	1673	CZ	PHE	A	119	10.769	4.130	46.209	1.00	26.61	C
ATOM	1675	CE2	PHE	A	119	10.678	5.519	46.220	1.00	27.63	C
ATOM	1677	CD2	PHE	A	119	11.667	6.262	46.824	1.00	27.28	C
ATOM	1679	C	PHE	A	119	15.992	7.509	47.867	1.00	31.21	C
ATOM	1680	O	PHE	A	119	16.326	7.269	49.011	1.00	30.42	O
ATOM	1681	N	THR	A	120	16.618	8.308	47.044	1.00	35.84	N
ATOM	1683	CA	THR	A	120	17.723	9.134	47.377	1.00	40.84	C
ATOM	1685	CB	THR	A	120	18.053	9.904	46.094	1.00	41.46	C
ATOM	1687	OG1	THR	A	120	19.173	9.271	45.454	1.00	42.35	O
ATOM	1689	CG2	THR	A	120	18.450	11.349	46.401	1.00	43.16	C
ATOM	1693	C	THR	A	120	17.403	10.086	48.525	1.00	43.46	C
ATOM	1694	O	THR	A	120	18.289	10.399	49.299	1.00	44.61	O
ATOM	1695	N	ASP	A	121	16.143	10.497	48.643	1.00	47.31	N
ATOM	1697	CA	ASP	A	121	15.737	11.435	49.695	1.00	50.01	C
ATOM	1699	CB	ASP	A	121	14.209	11.570	49.921	1.00	50.75	C
ATOM	1702	CG	ASP	A	121	13.347	11.236	48.704	1.00	54.79	C
ATOM	1703	OD1	ASP	A	121	13.846	11.206	47.551	1.00	61.49	O
ATOM	1704	OD2	ASP	A	121	12.110	11.008	48.825	1.00	58.98	O
ATOM	1705	C	ASP	A	121	16.286	10.928	51.009	1.00	51.36	C
ATOM	1706	O	ASP	A	121	16.965	11.661	51.735	1.00	51.86	O
ATOM	1707	N	LYS	A	122	15.972	9.676	51.318	1.00	51.80	N
ATOM	1709	CA	LYS	A	122	16.309	9.132	52.619	1.00	52.11	C
ATOM	1711	CB	LYS	A	122	15.685	7.758	52.788	1.00	52.52	C
ATOM	1714	CG	LYS	A	122	14.188	7.747	52.807	1.00	55.64	C
ATOM	1717	CD	LYS	A	122	13.696	6.497	53.547	1.00	59.67	C
ATOM	1720	CE	LYS	A	122	12.190	6.279	53.350	1.00	61.22	C
ATOM	1723	NZ	LYS	A	122	11.686	5.088	54.128	1.00	61.94	N
ATOM	1727	C	LYS	A	122	17.812	8.975	52.894	1.00	51.16	C
ATOM	1728	O	LYS	A	122	18.197	8.276	53.832	1.00	51.42	O

25/52

Figure 5-20

ATOM	1729	N	LEU	A	123	18.680	9.631	52.149	1.00	50.15	N
ATOM	1731	CA	LEU	A	123	20.108	9.391	52.368	1.00	48.71	C
ATOM	1733	CB	LEU	A	123	20.797	9.223	51.027	1.00	48.64	C
ATOM	1736	CG	LEU	A	123	20.440	7.988	50.196	1.00	46.77	C
ATOM	1738	CD1	LEU	A	123	21.470	7.818	49.115	1.00	45.94	C
ATOM	1742	CD2	LEU	A	123	20.343	6.768	51.084	1.00	45.63	C
ATOM	1746	C	LEU	A	123	20.868	10.471	53.167	1.00	48.55	C
ATOM	1747	O	LEU	A	123	20.386	11.571	53.291	1.00	47.82	O
ATOM	1748	N	PRO	A	124	21.957	10.099	53.847	1.00	48.08	N
ATOM	1749	CA	PRO	A	124	22.927	11.042	54.445	1.00	47.51	C
ATOM	1751	CB	PRO	A	124	24.107	10.120	54.818	1.00	48.23	C
ATOM	1754	CG	PRO	A	124	23.421	8.804	55.178	1.00	49.02	C
ATOM	1757	CD	PRO	A	124	22.123	8.748	54.403	1.00	48.73	C
ATOM	1760	C	PRO	A	124	23.333	12.280	53.568	1.00	46.05	C
ATOM	1761	O	PRO	A	124	23.871	12.133	52.466	1.00	44.21	O
ATOM	1762	N	LYS	A	125	23.102	13.498	54.090	1.00	45.42	N
ATOM	1764	CA	LYS	A	125	23.314	14.732	53.308	1.00	44.94	C
ATOM	1766	CB	LYS	A	125	23.090	16.025	54.084	1.00	46.11	C
ATOM	1769	CG	LYS	A	125	22.219	15.907	55.269	1.00	50.32	C
ATOM	1772	CD	LYS	A	125	20.784	16.363	54.959	1.00	54.20	C
ATOM	1775	CE	LYS	A	125	19.825	15.887	56.085	1.00	56.24	C
ATOM	1778	NZ	LYS	A	125	18.551	16.672	56.194	1.00	55.76	N
ATOM	1782	C	LYS	A	125	24.678	14.812	52.749	1.00	43.22	C
ATOM	1783	O	LYS	A	125	24.894	15.403	51.706	1.00	43.46	O
ATOM	1784	N	SER	A	126	25.644	14.219	53.386	1.00	40.92	N
ATOM	1786	CA	SER	A	126	26.903	14.331	52.735	1.00	39.77	C
ATOM	1788	CB	SER	A	126	28.046	14.354	53.730	1.00	41.05	C
ATOM	1791	OG	SER	A	126	28.288	13.069	54.239	1.00	41.88	O
ATOM	1793	C	SER	A	126	27.024	13.211	51.672	1.00	38.00	C
ATOM	1794	O	SER	A	126	27.828	13.318	50.762	1.00	37.20	O
ATOM	1795	N	THR	A	127	26.192	12.173	51.795	1.00	36.15	N
ATOM	1797	CA	THR	A	127	26.132	11.101	50.795	1.00	35.01	C
ATOM	1799	CB	THR	A	127	25.215	9.972	51.276	1.00	35.28	C
ATOM	1801	OG1	THR	A	127	25.586	9.517	52.613	1.00	37.62	O
ATOM	1803	CG2	THR	A	127	25.375	8.773	50.354	1.00	34.58	C
ATOM	1807	C	THR	A	127	25.506	11.683	49.524	1.00	33.00	C
ATOM	1808	O	THR	A	127	26.035	11.590	48.431	1.00	32.06	O
ATOM	1809	N	ILE	A	128	24.371	12.302	49.720	1.00	32.55	N
ATOM	1811	CA	ILE	A	128	23.634	12.936	48.632	1.00	33.42	C
ATOM	1813	CB	ILE	A	128	22.375	13.598	49.205	1.00	34.29	C
ATOM	1815	CG1	ILE	A	128	21.393	12.546	49.701	1.00	34.55	C
ATOM	1818	CD1	ILE	A	128	20.490	13.018	50.819	1.00	35.86	C
ATOM	1822	CG2	ILE	A	128	21.725	14.512	48.139	1.00	35.87	C
ATOM	1826	C	ILE	A	128	24.471	13.975	47.895	1.00	32.25	C
ATOM	1827	O	ILE	A	128	24.515	14.001	46.658	1.00	30.59	O

Figure 5-21

ATOM	1828	N	GLU A 129	25.142	14.845	48.650	1.00	32.15	N
ATOM	1830	CA	GLU A 129	25.949	15.880	48.018	1.00	32.23	C
ATOM	1832	CB	GLU A 129	26.544	16.821	49.065	1.00	32.98	C
ATOM	1835	CG	GLU A 129	25.430	17.577	49.805	1.00	37.27	C
ATOM	1838	CD	GLU A 129	25.898	18.689	50.728	1.00	43.34	C
ATOM	1839	OE1	GLU A 129	27.139	18.915	50.838	1.00	47.96	O
ATOM	1840	OE2	GLU A 129	25.003	19.346	51.342	1.00	43.81	O
ATOM	1841	C	GLU A 129	27.017	15.245	47.142	1.00	30.70	C
ATOM	1842	O	GLU A 129	27.261	15.677	46.047	1.00	28.60	O
ATOM	1843	N	ALA A 130	27.648	14.188	47.646	1.00	29.28	N
ATOM	1845	CA	ALA A 130	28.694	13.517	46.916	1.00	28.07	C
ATOM	1847	CB	ALA A 130	29.352	12.448	47.789	1.00	28.03	C
ATOM	1851	C	ALA A 130	28.100	12.877	45.641	1.00	26.91	C
ATOM	1852	O	ALA A 130	28.660	13.023	44.600	1.00	26.06	O
ATOM	1853	N	ILE A 131	26.985	12.175	45.777	1.00	26.72	N
ATOM	1855	CA	ILE A 131	26.310	11.547	44.626	1.00	27.04	C
ATOM	1857	CB	ILE A 131	25.087	10.755	45.137	1.00	27.32	C
ATOM	1859	CG1	ILE A 131	25.538	9.458	45.849	1.00	27.64	C
ATOM	1862	CD1	ILE A 131	24.482	8.940	46.729	1.00	29.11	C
ATOM	1866	CG2	ILE A 131	24.136	10.365	44.010	1.00	27.93	C
ATOM	1870	C	ILE A 131	25.920	12.620	43.563	1.00	26.60	C
ATOM	1871	O	ILE A 131	26.263	12.511	42.372	1.00	26.82	O
ATOM	1872	N	ASN A 132	25.260	13.680	44.020	1.00	26.44	N
ATOM	1874	CA	ASN A 132	24.846	14.787	43.120	1.00	27.52	C
ATOM	1876	CB	ASN A 132	24.052	15.821	43.917	1.00	27.47	C
ATOM	1879	CG	ASN A 132	22.609	15.391	44.141	1.00	30.87	C
ATOM	1880	OD1	ASN A 132	22.136	14.451	43.513	1.00	34.14	O
ATOM	1881	ND2	ASN A 132	21.904	16.085	45.026	1.00	31.65	N
ATOM	1884	C	ASN A 132	25.973	15.441	42.315	1.00	26.95	C
ATOM	1885	O	ASN A 132	25.819	15.696	41.119	1.00	26.30	O
ATOM	1886	N	ASN A 133	27.115	15.694	42.970	1.00	28.16	N
ATOM	1888	CA	ASN A 133	28.301	16.214	42.295	1.00	27.99	C
ATOM	1890	CB	ASN A 133	29.426	16.465	43.310	1.00	28.91	C
ATOM	1893	CG	ASN A 133	30.687	17.055	42.663	1.00	30.79	C
ATOM	1894	OD1	ASN A 133	30.679	18.179	42.185	1.00	32.81	O
ATOM	1895	ND2	ASN A 133	31.767	16.276	42.622	1.00	33.42	N
ATOM	1898	C	ASN A 133	28.792	15.265	41.188	1.00	27.08	C
ATOM	1899	O	ASN A 133	29.167	15.669	40.074	1.00	26.99	O
ATOM	1900	N	ALA A 134	28.889	13.973	41.505	1.00	26.84	N
ATOM	1902	CA	ALA A 134	29.287	13.023	40.486	1.00	26.24	C
ATOM	1904	CB	ALA A 134	29.487	11.631	41.082	1.00	26.73	C
ATOM	1908	C	ALA A 134	28.307	12.967	39.341	1.00	25.43	C
ATOM	1909	O	ALA A 134	28.710	12.892	38.199	1.00	24.70	O
ATOM	1910	N	LYS A 135	27.023	12.988	39.652	1.00	25.48	N

Figure 5-22

ATOM	1912	CA	LYS	A	135	26.012	13.026	38.616	1.00	26.60	C
ATOM	1914	CB	LYS	A	135	24.635	13.032	39.234	1.00	26.47	C
ATOM	1917	CG	LYS	A	135	24.189	11.700	39.805	1.00	27.64	C
ATOM	1920	CD	LYS	A	135	22.838	11.840	40.445	1.00	28.64	C
ATOM	1923	CE	LYS	A	135	22.119	10.542	40.658	1.00	32.99	C
ATOM	1926	NZ	LYS	A	135	20.658	10.847	40.900	1.00	33.57	N
ATOM	1930	C	LYS	A	135	26.231	14.304	37.779	1.00	28.10	C
ATOM	1931	O	LYS	A	135	26.263	14.255	36.559	1.00	26.96	O
ATOM	1932	N	GLU	A	136	26.442	15.423	38.459	1.00	30.14	N
ATOM	1934	CA	GLU	A	136	26.591	16.721	37.766	1.00	31.86	C
ATOM	1936	CB	GLU	A	136	26.646	17.851	38.788	1.00	33.63	C
ATOM	1939	CG	GLU	A	136	25.300	18.259	39.372	1.00	38.81	C
ATOM	1942	CD	GLU	A	136	25.424	19.220	40.545	1.00	45.39	C
ATOM	1943	OE1	GLU	A	136	26.538	19.738	40.770	1.00	50.00	O
ATOM	1944	OE2	GLU	A	136	24.414	19.449	41.248	1.00	49.83	O
ATOM	1945	C	GLU	A	136	27.821	16.772	36.859	1.00	31.26	C
ATOM	1946	O	GLU	A	136	27.732	17.192	35.689	1.00	30.86	O
ATOM	1947	N	LYS	A	137	28.967	16.335	37.382	1.00	30.48	N
ATOM	1949	CA	LYS	A	137	30.209	16.290	36.599	1.00	29.51	C
ATOM	1951	CB	LYS	A	137	31.416	16.023	37.509	1.00	29.97	C
ATOM	1954	CG	LYS	A	137	31.686	17.047	38.635	1.00	30.48	C
ATOM	1957	CD	LYS	A	137	31.769	18.491	38.150	1.00	32.50	C
ATOM	1960	CE	LYS	A	137	32.227	19.379	39.320	1.00	33.84	C
ATOM	1963	NZ	LYS	A	137	31.136	19.636	40.305	1.00	38.27	N
ATOM	1967	C	LYS	A	137	30.221	15.277	35.447	1.00	28.47	C
ATOM	1968	O	LYS	A	137	31.068	15.346	34.593	1.00	29.21	O
ATOM	1969	N	THR	A	138	29.310	14.310	35.430	1.00	27.31	N
ATOM	1971	CA	THR	A	138	29.294	13.301	34.390	1.00	26.62	C
ATOM	1973	CB	THR	A	138	29.466	11.874	35.001	1.00	25.85	C
ATOM	1975	OG1	THR	A	138	28.409	11.603	35.948	1.00	24.06	O
ATOM	1977	CG2	THR	A	138	30.747	11.806	35.852	1.00	26.39	C
ATOM	1981	C	THR	A	138	28.028	13.335	33.558	1.00	26.55	C
ATOM	1982	O	THR	A	138	27.863	12.515	32.709	1.00	26.31	O
ATOM	1983	N	ALA	A	139	27.155	14.306	33.808	1.00	28.34	N
ATOM	1985	CA	ALA	A	139	25.841	14.356	33.157	1.00	29.39	C
ATOM	1987	CB	ALA	A	139	25.066	15.541	33.659	1.00	30.19	C
ATOM	1991	C	ALA	A	139	25.826	14.351	31.642	1.00	29.63	C
ATOM	1992	O	ALA	A	139	24.832	13.928	31.064	1.00	30.80	O
ATOM	1993	N	ASN	A	140	26.897	14.818	31.005	1.00	30.37	N
ATOM	1995	CA	ASN	A	140	26.988	14.886	29.550	1.00	31.27	C
ATOM	1997	CB	ASN	A	140	27.483	16.294	29.154	1.00	32.75	C
ATOM	2000	CG	ASN	A	140	26.479	17.375	29.512	1.00	33.74	C
ATOM	2001	OD1	ASN	A	140	25.253	17.152	29.457	1.00	37.70	O
ATOM	2002	ND2	ASN	A	140	26.973	18.541	29.880	1.00	38.58	N
ATOM	2005	C	ASN	A	140	27.872	13.777	28.922	1.00	31.79	C

Figure S-23

ATOM	2006	O	ASN	A	140	28.111	13.740	27.710	1.00	31.16	O
ATOM	2007	N	ASN	A	141	28.367	12.860	29.762	1.00	30.17	N
ATOM	2009	CA	ASN	A	141	29.111	11.727	29.268	1.00	28.98	C
ATOM	2011	CB	ASN	A	141	29.786	11.022	30.429	1.00	28.17	C
ATOM	2014	CG	ASN	A	141	30.920	11.828	31.038	1.00	30.41	C
ATOM	2015	OD1	ASN	A	141	31.498	11.420	32.050	1.00	27.02	O
ATOM	2016	ND2	ASN	A	141	31.289	12.952	30.398	1.00	28.83	N
ATOM	2019	C	ASN	A	141	28.219	10.760	28.525	1.00	27.39	C
ATOM	2020	O	ASN	A	141	27.074	10.528	28.914	1.00	28.15	O
ATOM	2021	N	THR	A	142	28.761	10.143	27.494	1.00	25.05	N
ATOM	2023	CA	THR	A	142	27.995	9.312	26.600	1.00	25.00	C
ATOM	2025	CB	THR	A	142	28.076	9.884	25.147	1.00	26.25	C
ATOM	2027	OG1	THR	A	142	29.435	9.880	24.721	1.00	26.97	O
ATOM	2029	CG2	THR	A	142	27.689	11.362	25.128	1.00	28.81	C
ATOM	2033	C	THR	A	142	28.453	7.885	26.586	1.00	23.01	C
ATOM	2034	O	THR	A	142	28.031	7.138	25.760	1.00	23.31	O
ATOM	2035	N	GLY	A	143	29.285	7.471	27.524	1.00	22.23	N
ATOM	2037	CA	GLY	A	143	29.665	6.063	27.554	1.00	20.41	C
ATOM	2040	C	GLY	A	143	28.832	5.251	28.540	1.00	20.61	C
ATOM	2041	O	GLY	A	143	27.628	5.526	28.752	1.00	21.12	O
ATOM	2042	N	LEU	A	144	29.464	4.252	29.172	1.00	19.99	N
ATOM	2044	CA	LEU	A	144	28.774	3.433	30.176	1.00	18.97	C
ATOM	2046	CB	LEU	A	144	29.761	2.573	30.951	1.00	18.88	C
ATOM	2049	CG	LEU	A	144	29.173	1.772	32.139	1.00	19.88	C
ATOM	2051	CD1	LEU	A	144	28.469	0.585	31.617	1.00	18.36	C
ATOM	2055	CD2	LEU	A	144	30.371	1.381	33.083	1.00	20.07	C
ATOM	2059	C	LEU	A	144	27.961	4.245	31.160	1.00	17.92	C
ATOM	2060	O	LEU	A	144	28.424	5.265	31.690	1.00	19.14	O
ATOM	2061	N	LYS	A	145	26.716	3.806	31.394	1.00	17.70	N
ATOM	2063	CA	LYS	A	145	25.885	4.357	32.433	1.00	17.79	C
ATOM	2065	CB	LYS	A	145	24.399	4.413	32.009	1.00	18.98	C
ATOM	2068	CG	LYS	A	145	24.158	5.593	31.015	1.00	22.40	C
ATOM	2071	CD	LYS	A	145	22.712	5.912	30.687	1.00	26.05	C
ATOM	2074	CE	LYS	A	145	22.656	6.883	29.493	1.00	29.57	C
ATOM	2077	NZ	LYS	A	145	21.275	6.825	28.891	1.00	37.07	N
ATOM	2081	C	LYS	A	145	26.071	3.467	33.647	1.00	17.90	C
ATOM	2082	O	LYS	A	145	25.724	2.306	33.595	1.00	18.27	O
ATOM	2083	N	LEU	A	146	26.745	4.017	34.654	1.00	16.64	N
ATOM	2085	CA	LEU	A	146	26.998	3.306	35.946	1.00	16.08	C
ATOM	2087	CB	LEU	A	146	28.315	3.748	36.516	1.00	16.46	C
ATOM	2090	CG	LEU	A	146	28.735	3.124	37.856	1.00	17.84	C
ATOM	2092	CD1	LEU	A	146	28.714	1.640	37.693	1.00	15.64	C
ATOM	2096	CD2	LEU	A	146	30.132	3.597	38.261	1.00	18.63	C
ATOM	2100	C	LEU	A	146	25.913	3.711	36.875	1.00	14.86	C
ATOM	2101	O	LEU	A	146	25.839	4.859	37.314	1.00	14.43	O

Figure 5-24

ATOM	2102	N	ILE A 147	25.037	2.768	37.170	1.00	15.31	N
ATOM	2104	CA	ILE A 147	23.841	3.012	37.914	1.00	14.03	C
ATOM	2106	CB	ILE A 147	22.667	2.448	37.113	1.00	15.45	C
ATOM	2108	CG1	ILE A 147	22.622	3.069	35.705	1.00	17.02	C
ATOM	2111	CD1	ILE A 147	21.884	2.188	34.686	1.00	16.53	C
ATOM	2115	CG2	ILE A 147	21.356	2.760	37.776	1.00	17.34	C
ATOM	2119	C	ILE A 147	23.860	2.369	39.287	1.00	15.48	C
ATOM	2120	O	ILE A 147	23.806	1.131	39.386	1.00	14.27	O
ATOM	2121	N	PHE A 148	23.877	3.190	40.337	1.00	15.33	N
ATOM	2123	CA	PHE A 148	23.853	2.680	41.714	1.00	15.28	C
ATOM	2125	CB	PHE A 148	24.708	3.555	42.622	1.00	15.14	C
ATOM	2128	CG	PHE A 148	26.175	3.566	42.273	1.00	17.86	C
ATOM	2129	CD1	PHE A 148	26.981	2.484	42.609	1.00	22.24	C
ATOM	2131	CE1	PHE A 148	28.322	2.479	42.242	1.00	24.27	C
ATOM	2133	CZ	PHE A 148	28.863	3.572	41.594	1.00	25.59	C
ATOM	2135	CE2	PHE A 148	28.090	4.625	41.269	1.00	23.93	C
ATOM	2137	CD2	PHE A 148	26.753	4.628	41.601	1.00	20.24	C
ATOM	2139	C	PHE A 148	22.421	2.603	42.224	1.00	15.00	C
ATOM	2140	O	PHE A 148	21.733	3.581	42.230	1.00	15.07	O
ATOM	2141	N	ALA A 149	21.983	1.403	42.621	1.00	14.72	N
ATOM	2143	CA	ALA A 149	20.709	1.185	43.242	1.00	14.17	C
ATOM	2145	CB	ALA A 149	20.194	-0.151	42.913	1.00	14.78	C
ATOM	2149	C	ALA A 149	20.866	1.295	44.759	1.00	15.52	C
ATOM	2150	O	ALA A 149	21.249	0.316	45.388	1.00	16.47	O
ATOM	2151	N	ILE A 150	20.562	2.466	45.295	1.00	16.74	N
ATOM	2153	CA	ILE A 150	20.790	2.844	46.686	1.00	18.03	C
ATOM	2155	CB	ILE A 150	21.775	4.024	46.787	1.00	19.24	C
ATOM	2157	CG1	ILE A 150	23.045	3.774	46.014	1.00	23.93	C
ATOM	2160	CD1	ILE A 150	23.974	5.019	45.901	1.00	27.20	C
ATOM	2164	CG2	ILE A 150	22.200	4.172	48.247	1.00	21.30	C
ATOM	2168	C	ILE A 150	19.467	3.236	47.348	1.00	17.53	C
ATOM	2169	O	ILE A 150	18.755	4.144	46.879	1.00	18.10	O
ATOM	2170	N	ASN A 151	19.124	2.528	48.412	1.00	17.27	N
ATOM	2172	CA	ASN A 151	17.808	2.610	49.035	1.00	18.05	C
ATOM	2174	CB	ASN A 151	17.549	3.934	49.689	1.00	19.07	C
ATOM	2177	CG	ASN A 151	16.339	3.883	50.591	1.00	21.11	C
ATOM	2178	OD1	ASN A 151	15.987	2.814	51.090	1.00	20.31	O
ATOM	2179	ND2	ASN A 151	15.724	5.048	50.855	1.00	22.15	N
ATOM	2182	C	ASN A 151	16.757	2.310	47.990	1.00	18.97	C
ATOM	2183	O	ASN A 151	15.801	3.073	47.814	1.00	19.79	O
ATOM	2184	N	TYR A 152	16.960	1.169	47.300	1.00	17.97	N
ATOM	2186	CA	TYR A 152	16.145	0.735	46.181	1.00	17.14	C

Figure 5-25

ATOM	2188	CB	TYR	A	152	17.014	0.589	44.932	1.00	16.30	C
ATOM	2191	CG	TYR	A	152	16.214	-0.098	43.854	1.00	17.01	C
ATOM	2192	CD1	TYR	A	152	15.334	0.599	43.061	1.00	16.08	C
ATOM	2194	CE1	TYR	A	152	14.606	-0.004	42.106	1.00	13.74	C
ATOM	2196	CZ	TYR	A	152	14.652	-1.342	41.984	1.00	16.95	C
ATOM	2197	OH	TYR	A	152	13.879	-1.922	41.002	1.00	19.37	O
ATOM	2199	CE2	TYR	A	152	15.514	-2.061	42.742	1.00	17.81	C
ATOM	2201	CD2	TYR	A	152	16.258	-1.440	43.715	1.00	16.89	C
ATOM	2203	C	TYR	A	152	15.517	-0.609	46.495	1.00	17.42	C
ATOM	2204	O	TYR	A	152	16.147	-1.413	47.154	1.00	15.67	O
ATOM	2205	N	GLY	A	153	14.273	-0.811	46.063	1.00	16.45	N
ATOM	2207	CA	GLY	A	153	13.582	-2.063	46.246	1.00	16.91	C
ATOM	2210	C	GLY	A	153	12.524	-2.117	45.153	1.00	16.43	C
ATOM	2211	O	GLY	A	153	11.922	-1.078	44.816	1.00	15.62	O
ATOM	2212	N	GLY	A	154	12.362	-3.259	44.505	1.00	13.23	N
ATOM	2214	CA	GLY	A	154	11.391	-3.361	43.444	1.00	15.77	C
ATOM	2217	C	GLY	A	154	9.956	-3.147	43.858	1.00	15.88	C
ATOM	2218	O	GLY	A	154	9.179	-2.495	43.118	1.00	17.22	O
ATOM	2219	N	ARG	A	155	9.591	-3.685	44.996	1.00	17.38	N
ATOM	2221	CA	ARG	A	155	8.223	-3.520	45.442	1.00	18.28	C
ATOM	2223	CB	ARG	A	155	7.985	-4.327	46.660	1.00	19.82	C
ATOM	2226	CG	ARG	A	155	7.637	-5.793	46.321	1.00	19.33	C
ATOM	2229	CD	ARG	A	155	7.341	-6.590	47.522	1.00	19.68	C
ATOM	2232	NE	ARG	A	155	7.048	-7.981	47.152	1.00	17.70	N
ATOM	2234	CZ	ARG	A	155	6.421	-8.832	47.917	1.00	21.19	C
ATOM	2235	NH1	ARG	A	155	6.084	-8.488	49.141	1.00	22.37	N
ATOM	2238	NH2	ARG	A	155	6.182	-10.057	47.487	1.00	19.80	N
ATOM	2241	C	ARG	A	155	7.968	-2.007	45.737	1.00	19.50	C
ATOM	2242	O	ARG	A	155	6.991	-1.446	45.273	1.00	19.06	O
ATOM	2243	N	ALA	A	156	8.931	-1.351	46.367	1.00	18.85	N
ATOM	2245	CA	ALA	A	156	8.822	0.085	46.694	1.00	19.21	C
ATOM	2247	CB	ALA	A	156	9.901	0.493	47.685	1.00	20.79	C
ATOM	2251	C	ALA	A	156	8.818	0.950	45.451	1.00	20.44	C
ATOM	2252	O	ALA	A	156	8.078	1.955	45.407	1.00	21.72	O
ATOM	2253	N	GLU	A	157	9.607	0.585	44.429	1.00	19.55	N
ATOM	2255	CA	GLU	A	157	9.639	1.249	43.140	1.00	20.66	C
ATOM	2257	CB	GLU	A	157	10.635	0.593	42.159	1.00	18.64	C
ATOM	2260	CG	GLU	A	157	10.527	1.073	40.713	1.00	22.36	C
ATOM	2263	CD	GLU	A	157	11.539	0.447	39.769	1.00	17.16	C
ATOM	2264	OE1	GLU	A	157	11.919	-0.767	39.961	1.00	18.55	O
ATOM	2265	OE2	GLU	A	157	11.981	1.141	38.814	1.00	20.62	O
ATOM	2266	C	GLU	A	157	8.267	1.180	42.499	1.00	21.44	C
ATOM	2267	O	GLU	A	157	7.776	2.181	41.966	1.00	21.31	O
ATOM	2268	N	LEU	A	158	7.669	-0.006	42.498	1.00	20.86	N
ATOM	2270	CA	LEU	A	158	6.356	-0.167	41.896	1.00	21.83	C
ATOM	2272	CB	LEU	A	158	5.948	-1.646	41.829	1.00	21.43	C
ATOM	2275	CG	LEU	A	158	6.424	-2.322	40.552	1.00	21.25	C
ATOM	2277	CD1	LEU	A	158	6.615	-3.840	40.785	1.00	21.37	C
ATOM	2281	CD2	LEU	A	158	5.569	-2.086	39.351	1.00	22.07	C

Figure 5-26

ATOM	2285	C	LEU	A	158	5.274	0.627	42.622	1.00	23.95	C
ATOM	2286	O	LEU	A	158	4.410	1.232	41.958	1.00	24.54	O
ATOM	2287	N	VAL	A	159	5.317	0.611	43.941	1.00	25.78	N
ATOM	2289	CA	VAL	A	159	4.327	1.308	44.746	1.00	28.05	C
ATOM	2291	CB	VAL	A	159	4.557	1.079	46.222	1.00	28.19	C
ATOM	2293	CG1	VAL	A	159	3.811	2.079	47.095	1.00	30.63	C
ATOM	2297	CG2	VAL	A	159	4.108	-0.318	46.630	1.00	27.07	C
ATOM	2301	C	VAL	A	159	4.401	2.806	44.369	1.00	29.71	C
ATOM	2302	O	VAL	A	159	3.389	3.454	44.036	1.00	28.90	O
ATOM	2303	N	HIS	A	160	5.606	3.340	44.452	1.00	29.66	N
ATOM	2305	CA	HIS	A	160	5.856	4.729	44.095	1.00	31.05	C
ATOM	2307	CB	HIS	A	160	7.353	5.012	44.221	1.00	30.62	C
ATOM	2310	CG	HIS	A	160	7.698	6.438	43.988	1.00	31.39	C
ATOM	2311	ND1	HIS	A	160	8.199	6.893	42.788	1.00	32.63	N
ATOM	2313	CE1	HIS	A	160	8.402	8.195	42.868	1.00	30.14	C
ATOM	2315	NE2	HIS	A	160	8.010	8.604	44.060	1.00	29.50	N
ATOM	2317	CD2	HIS	A	160	7.556	7.527	44.780	1.00	31.56	C
ATOM	2319	C	HIS	A	160	5.389	5.094	42.697	1.00	32.15	C
ATOM	2320	O	HIS	A	160	4.623	6.073	42.563	1.00	33.83	O
ATOM	2321	N	SER	A	161	5.826	4.319	41.692	1.00	31.48	N
ATOM	2323	CA	SER	A	161	5.505	4.472	40.262	1.00	32.90	C
ATOM	2325	CB	SER	A	161	6.093	3.371	39.374	1.00	32.79	C
ATOM	2328	OG	SER	A	161	7.480	3.587	39.115	1.00	31.01	O
ATOM	2330	C	SER	A	161	3.970	4.512	40.116	1.00	34.85	C
ATOM	2331	O	SER	A	161	3.415	5.243	39.256	1.00	33.91	O
ATOM	2332	N	ILE	A	162	3.323	3.752	41.013	1.00	35.77	N
ATOM	2334	CA	ILE	A	162	1.866	3.589	41.065	1.00	38.69	C
ATOM	2336	CB	ILE	A	162	1.483	2.268	41.696	1.00	37.84	C
ATOM	2338	CG1	ILE	A	162	1.796	1.164	40.721	1.00	36.97	C
ATOM	2341	CD1	ILE	A	162	2.036	-0.126	41.402	1.00	34.12	C
ATOM	2345	CG2	ILE	A	162	0.004	2.197	42.038	1.00	38.58	C
ATOM	2349	C	ILE	A	162	1.108	4.685	41.796	1.00	39.81	C
ATOM	2350	O	ILE	A	162	0.233	5.242	41.192	1.00	40.71	O
ATOM	2351	N	LYS	A	163	1.407	4.979	43.069	1.00	41.77	N
ATOM	2353	CA	LYS	A	163	0.677	6.070	43.767	1.00	43.30	C
ATOM	2355	CB	LYS	A	163	1.262	6.462	45.116	1.00	43.09	C
ATOM	2358	CG	LYS	A	163	1.431	5.392	46.114	1.00	43.32	C
ATOM	2361	CD	LYS	A	163	1.801	5.991	47.447	1.00	45.79	C
ATOM	2364	CE	LYS	A	163	2.207	4.915	48.417	1.00	46.66	C
ATOM	2367	NZ	LYS	A	163	1.671	5.127	49.807	1.00	47.62	N
ATOM	2371	C	LYS	A	163	0.893	7.267	42.909	1.00	44.45	C
ATOM	2372	O	LYS	A	163	0.648	8.399	43.312	1.00	46.11	O
ATOM	2373	N	ASN	A	164	1.297	6.994	41.693	1.00	46.06	N
ATOM	2375	CA	ASN	A	164	1.830	8.009	40.842	1.00	46.83	C
ATOM	2377	CB	ASN	A	164	3.284	7.630	40.772	1.00	47.88	C
ATOM	2380	CG	ASN	A	164	4.197	8.787	40.674	1.00	51.87	C
ATOM	2381	OD1	ASN	A	164	5.301	8.643	40.167	1.00	60.08	O
ATOM	2382	ND2	ASN	A	164	3.820	9.890	41.222	1.00	53.56	N
ATOM	2385	C	ASN	A	164	1.257	8.149	39.403	1.00	46.61	C

Figure 5-27

ATOM	2386	O	ASN A 164	0.618	9.169	39.103	1.00	47.72	O
ATOM	2387	N	MET A 165	1.557	7.186	38.508	1.00	44.51	N
ATOM	2389	CA	MET A 165	1.071	7.148	37.106	1.00	42.30	C
ATOM	2391	CB	MET A 165	0.961	5.710	36.604	1.00	42.43	C
ATOM	2394	CG	MET A 165	2.209	5.048	36.219	1.00	44.44	C
ATOM	2397	SE	MET A 165	1.897	3.252	35.722	1.00	45.39	SE
ATOM	2398	CE	MET A 165	1.896	2.517	37.491	1.00	46.30	C
ATOM	2402	C	MET A 165	-0.339	7.626	37.108	1.00	39.71	C
ATOM	2403	O	MET A 165	-0.874	8.178	36.131	1.00	37.61	O
ATOM	2404	N	PHE A 166	-0.925	7.328	38.250	1.00	36.75	N
ATOM	2406	CA	PHE A 166	-2.261	7.643	38.547	1.00	36.32	C
ATOM	2408	CB	PHE A 166	-2.487	7.299	40.020	1.00	37.46	C
ATOM	2411	CG	PHE A 166	-3.315	8.345	40.691	1.00	42.82	C
ATOM	2412	CD1	PHE A 166	-4.636	8.443	40.376	1.00	47.35	C
ATOM	2414	CE1	PHE A 166	-5.390	9.406	40.905	1.00	50.37	C
ATOM	2416	CZ	PHE A 166	-4.842	10.349	41.749	1.00	51.55	C
ATOM	2418	CE2	PHE A 166	-3.506	10.286	42.059	1.00	50.20	C
ATOM	2420	CD2	PHE A 166	-2.733	9.285	41.518	1.00	46.62	C
ATOM	2422	C	PHE A 166	-2.506	9.162	38.319	1.00	35.46	C
ATOM	2423	O	PHE A 166	-3.454	9.635	37.602	1.00	31.59	O
ATOM	2424	N	ASP A 167	-1.654	9.955	38.954	1.00	35.14	N
ATOM	2426	CA	ASP A 167	-1.768	11.401	38.849	1.00	35.58	C
ATOM	2428	CB	ASP A 167	-0.775	12.059	39.802	1.00	35.84	C
ATOM	2431	CG	ASP A 167	-0.866	13.580	39.776	1.00	38.35	C
ATOM	2432	OD1	ASP A 167	0.185	14.225	39.527	1.00	38.02	O
ATOM	2433	OD2	ASP A 167	-1.930	14.193	39.991	1.00	38.15	O
ATOM	2434	C	ASP A 167	-1.550	11.846	37.421	1.00	36.25	C
ATOM	2435	O	ASP A 167	-2.286	12.711	36.913	1.00	37.31	O
ATOM	2436	N	GLU A 168	-0.589	11.239	36.734	1.00	37.00	N
ATOM	2438	CA	GLU A 168	-0.342	11.570	35.334	1.00	38.95	C
ATOM	2440	CB	GLU A 168	0.902	10.830	34.798	1.00	39.48	C
ATOM	2443	CG	GLU A 168	1.488	11.411	33.519	1.00	40.34	C
ATOM	2446	CD	GLU A 168	2.731	10.675	33.018	1.00	39.95	C
ATOM	2447	OE1	GLU A 168	3.775	10.690	33.717	1.00	42.15	O
ATOM	2448	OE2	GLU A 168	2.659	10.080	31.913	1.00	39.19	O
ATOM	2449	C	GLU A 168	-1.597	11.355	34.437	1.00	41.21	C
ATOM	2450	O	GLU A 168	-2.091	12.335	33.870	1.00	41.39	O
ATOM	2451	N	LEU A 169	-2.097	10.123	34.259	1.00	43.08	N
ATOM	2453	CA	LEU A 169	-3.292	9.900	33.400	1.00	45.13	C
ATOM	2455	CB	LEU A 169	-3.956	8.535	33.680	1.00	45.35	C
ATOM	2458	CG	LEU A 169	-3.060	7.289	33.697	1.00	47.82	C
ATOM	2460	CD1	LEU A 169	-3.827	6.079	34.246	1.00	48.92	C
ATOM	2464	CD2	LEU A 169	-2.503	6.994	32.324	1.00	49.01	C
ATOM	2468	C	LEU A 169	-4.323	11.027	33.623	1.00	46.44	C
ATOM	2469	O	LEU A 169	-4.741	11.748	32.689	1.00	47.30	O
ATOM	2470	N	HIS A 170	-4.735	11.115	34.886	1.00	47.15	N
ATOM	2472	CA	HIS A 170	-5.625	12.125	35.463	1.00	48.07	C
ATOM	2474	CB	HIS A 170	-5.327	12.112	36.967	1.00	48.83	C
ATOM	2477	CG	HIS A 170	-6.401	11.519	37.822	1.00	51.25	C

Figure 5-28

ATOM	2478	ND1	HIS	A	170	-6.224	11.304	39.173	1.00	52.95	N
ATOM	2480	CE1	HIS	A	170	-7.342	10.835	39.696	1.00	54.48	C
ATOM	2482	NE2	HIS	A	170	-8.240	10.730	38.735	1.00	54.28	N
ATOM	2484	CD2	HIS	A	170	-7.680	11.160	37.553	1.00	55.68	C
ATOM	2486	C	HIS	A	170	-5.447	13.579	34.904	1.00	47.74	C
ATOM	2487	O	HIS	A	170	-6.310	14.153	34.239	1.00	46.55	O
ATOM	2488	N	GLN	A	171	-4.310	14.173	35.211	1.00	48.24	N
ATOM	2490	CA	GLN	A	171	-4.003	15.517	34.754	1.00	49.07	C
ATOM	2492	CB	GLN	A	171	-2.622	15.919	35.269	1.00	48.64	C
ATOM	2495	CG	GLN	A	171	-2.526	15.809	36.787	1.00	47.10	C
ATOM	2498	CD	GLN	A	171	-3.639	16.571	37.478	1.00	45.14	C
ATOM	2499	OE1	GLN	A	171	-4.328	17.407	36.848	1.00	39.58	O
ATOM	2500	NE2	GLN	A	171	-3.841	16.275	38.765	1.00	41.59	N
ATOM	2503	C	GLN	A	171	-4.053	15.679	33.235	1.00	50.41	C
ATOM	2504	O	GLN	A	171	-4.031	16.808	32.739	1.00	49.74	O
ATOM	2505	N	GLN	A	172	-4.167	14.563	32.508	1.00	51.89	N
ATOM	2507	CA	GLN	A	172	-4.160	14.599	31.049	1.00	53.77	C
ATOM	2509	CB	GLN	A	172	-3.111	13.610	30.528	1.00	53.91	C
ATOM	2512	CG	GLN	A	172	-1.695	13.899	30.918	1.00	55.27	C
ATOM	2515	CD	GLN	A	172	-0.751	13.307	29.899	1.00	58.84	C
ATOM	2516	OE1	GLN	A	172	-1.202	12.771	28.884	1.00	60.19	O
ATOM	2517	NE2	GLN	A	172	0.555	13.412	30.146	1.00	61.41	N
ATOM	2520	C	GLN	A	172	-5.458	14.202	30.353	1.00	54.91	C
ATOM	2521	O	GLN	A	172	-5.557	14.297	29.137	1.00	55.17	O
ATOM	2522	N	GLY	A	173	-6.452	13.748	31.094	1.00	56.49	N
ATOM	2524	CA	GLY	A	173	-7.587	13.101	30.449	1.00	57.73	C
ATOM	2527	C	GLY	A	173	-7.138	11.639	30.469	1.00	58.51	C
ATOM	2528	O	GLY	A	173	-5.961	11.367	30.239	1.00	58.72	O
ATOM	2529	N	LEU	A	174	-8.025	10.682	30.717	1.00	59.79	N
ATOM	2531	CA	LEU	A	174	-7.485	9.376	31.113	1.00	60.28	C
ATOM	2533	CB	LEU	A	174	-7.314	9.506	32.635	1.00	60.17	C
ATOM	2536	CG	LEU	A	174	-8.243	10.572	33.239	1.00	60.12	C
ATOM	2538	CD1	LEU	A	174	-9.175	10.106	34.340	1.00	59.93	C
ATOM	2542	CD2	LEU	A	174	-7.373	11.631	33.742	1.00	60.49	C
ATOM	2546	C	LEU	A	174	-8.089	7.983	31.057	1.00	60.71	C
ATOM	2547	O	LEU	A	174	-9.078	7.632	30.415	1.00	61.69	O
ATOM	2548	N	ASN	A	175	-7.285	7.215	31.775	1.00	60.96	N
ATOM	2550	CA	ASN	A	175	-7.524	5.954	32.425	1.00	60.73	C
ATOM	2552	CB	ASN	A	175	-8.601	6.003	33.488	1.00	61.29	C
ATOM	2555	CG	ASN	A	175	-8.015	5.712	34.843	1.00	62.29	C
ATOM	2556	OD1	ASN	A	175	-6.797	5.761	35.010	1.00	66.10	O
ATOM	2557	ND2	ASN	A	175	-8.843	5.370	35.794	1.00	63.44	N
ATOM	2560	C	ASN	A	175	-7.359	4.591	31.937	1.00	59.54	C
ATOM	2561	O	ASN	A	175	-7.821	4.124	30.905	1.00	60.86	O
ATOM	2562	N	SER	A	176	-6.648	3.966	32.850	1.00	58.11	N
ATOM	2564	CA	SER	A	176	-6.324	2.600	32.863	1.00	56.33	C
ATOM	2566	CB	SER	A	176	-7.428	1.880	33.609	1.00	56.27	C
ATOM	2569	OG	SER	A	176	-8.638	1.864	32.878	1.00	55.01	O
ATOM	2571	C	SER	A	176	-6.143	2.135	31.449	1.00	55.62	C

Figure 5-29

ATOM	2572	O	SER	A	176	-5.118	1.588	31.099	1.00	54.86	O
ATOM	2573	N	ASP	A	177	-7.110	2.395	30.605	1.00	54.36	N
ATOM	2575	CA	ASP	A	177	-6.987	1.870	29.274	1.00	54.51	C
ATOM	2577	CB	ASP	A	177	-8.239	2.201	28.471	1.00	54.94	C
ATOM	2580	CG	ASP	A	177	-9.486	1.529	29.087	1.00	56.25	C
ATOM	2581	OD1	ASP	A	177	-9.360	0.996	30.227	1.00	59.54	O
ATOM	2582	OD2	ASP	A	177	-10.601	1.457	28.528	1.00	57.47	O
ATOM	2583	C	ASP	A	177	-5.647	2.289	28.680	1.00	53.70	C
ATOM	2584	O	ASP	A	177	-5.097	1.592	27.820	1.00	53.46	O
ATOM	2585	N	ILE	A	178	-5.100	3.398	29.185	1.00	53.22	N
ATOM	2587	CA	ILE	A	178	-3.736	3.806	28.840	1.00	52.58	C
ATOM	2589	CB	ILE	A	178	-3.487	5.291	29.138	1.00	52.65	C
ATOM	2591	CG1	ILE	A	178	-4.345	6.183	28.240	1.00	55.38	C
ATOM	2594	CD1	ILE	A	178	-3.973	6.094	26.742	1.00	57.52	C
ATOM	2598	CG2	ILE	A	178	-2.005	5.657	28.903	1.00	53.54	C
ATOM	2602	C	ILE	A	178	-2.719	2.964	29.634	1.00	50.54	C
ATOM	2603	O	ILE	A	178	-1.529	2.986	29.375	1.00	51.48	O
ATOM	2604	N	ILE	A	179	-3.161	2.227	30.618	1.00	49.04	N
ATOM	2606	CA	ILE	A	179	-2.192	1.430	31.345	1.00	47.21	C
ATOM	2608	CB	ILE	A	179	-2.620	1.271	32.745	1.00	47.24	C
ATOM	2610	CG1	ILE	A	179	-2.507	2.612	33.420	1.00	45.34	C
ATOM	2613	CD1	ILE	A	179	-3.239	2.696	34.659	1.00	44.29	C
ATOM	2617	CG2	ILE	A	179	-1.729	0.269	33.475	1.00	48.09	C
ATOM	2621	C	ILE	A	179	-1.983	0.113	30.643	1.00	46.08	C
ATOM	2622	O	ILE	A	179	-2.922	-0.578	30.301	1.00	46.78	O
ATOM	2623	N	ASP	A	180	-0.732	-0.196	30.363	1.00	43.84	N
ATOM	2625	CA	ASP	A	180	-0.358	-1.466	29.762	1.00	42.42	C
ATOM	2627	CB	ASP	A	180	-0.417	-1.396	28.268	1.00	42.25	C
ATOM	2630	CG	ASP	A	180	0.392	-0.282	27.746	1.00	44.62	C
ATOM	2631	OD1	ASP	A	180	0.625	0.650	28.558	1.00	45.57	O
ATOM	2632	OD2	ASP	A	180	0.821	-0.252	26.580	1.00	43.92	O
ATOM	2633	C	ASP	A	180	1.057	-1.746	30.221	1.00	40.07	C
ATOM	2634	O	ASP	A	180	1.533	-1.048	31.105	1.00	39.80	O
ATOM	2635	N	GLU	A	181	1.737	-2.706	29.588	1.00	38.18	N
ATOM	2637	CA	GLU	A	181	3.066	-3.161	30.049	1.00	35.76	C
ATOM	2639	CB	GLU	A	181	3.398	-4.588	29.521	1.00	34.99	C
ATOM	2642	CG	GLU	A	181	2.700	-5.729	30.304	1.00	34.67	C
ATOM	2645	CD	GLU	A	181	2.941	-7.163	29.776	1.00	32.43	C
ATOM	2646	OE1	GLU	A	181	4.092	-7.425	29.301	1.00	25.34	O
ATOM	2647	OE2	GLU	A	181	1.970	-8.048	29.845	1.00	25.96	O
ATOM	2648	C	GLU	A	181	4.120	-2.095	29.688	1.00	35.34	C
ATOM	2649	O	GLU	A	181	4.809	-1.595	30.574	1.00	35.04	O
ATOM	2650	N	THR	A	182	4.157	-1.701	28.415	1.00	34.48	N
ATOM	2652	CA	THR	A	182	5.067	-0.684	27.872	1.00	34.75	C
ATOM	2654	CB	THR	A	182	4.744	-0.503	26.346	1.00	34.50	C
ATOM	2656	OG1	THR	A	182	5.230	-1.630	25.600	1.00	36.93	O
ATOM	2658	CG2	THR	A	182	5.512	0.655	25.705	1.00	36.22	C
ATOM	2662	C	THR	A	182	4.952	0.634	28.672	1.00	33.46	C
ATOM	2663	O	THR	A	182	5.955	1.289	29.025	1.00	33.84	O

Figure S-30

ATOM	2664	N	TYR	A	183	3.729	1.009	28.994	1.00	32.75	N
ATOM	2666	CA	TYR	A	183	3.469	2.175	29.839	1.00	31.80	C
ATOM	2668	CB	TYR	A	183	1.967	2.302	30.101	1.00	32.74	C
ATOM	2671	CG	TYR	A	183	1.531	3.615	30.667	1.00	33.08	C
ATOM	2672	CD1	TYR	A	183	1.457	4.743	29.845	1.00	36.08	C
ATOM	2674	CE1	TYR	A	183	1.065	5.958	30.354	1.00	35.88	C
ATOM	2676	CZ	TYR	A	183	0.725	6.064	31.673	1.00	33.84	C
ATOM	2677	OH	TYR	A	183	0.358	7.300	32.158	1.00	38.24	O
ATOM	2679	CE2	TYR	A	183	0.799	4.958	32.518	1.00	34.80	C
ATOM	2681	CD2	TYR	A	183	1.168	3.753	32.002	1.00	30.93	C
ATOM	2683	C	TYR	A	183	4.145	2.039	31.195	1.00	31.82	C
ATOM	2684	O	TYR	A	183	4.728	3.000	31.727	1.00	31.30	O
ATOM	2685	N	ILE	A	184	4.036	0.853	31.790	1.00	29.02	N
ATOM	2687	CA	ILE	A	184	4.656	0.670	33.085	1.00	28.77	C
ATOM	2689	CB	ILE	A	184	4.303	-0.697	33.711	1.00	28.03	C
ATOM	2691	CG1	ILE	A	184	2.786	-0.828	33.814	1.00	30.47	C
ATOM	2694	CD1	ILE	A	184	2.217	-0.024	34.908	1.00	31.42	C
ATOM	2698	CG2	ILE	A	184	4.923	-0.861	35.121	1.00	27.80	C
ATOM	2702	C	ILE	A	184	6.132	0.808	32.862	1.00	26.59	C
ATOM	2703	O	ILE	A	184	6.762	1.520	33.623	1.00	28.92	O
ATOM	2704	N	ASN	A	185	6.675	0.168	31.826	1.00	26.01	N
ATOM	2706	CA	ASN	A	185	8.117	0.299	31.515	1.00	27.03	C
ATOM	2708	CB	ASN	A	185	8.479	-0.265	30.168	1.00	27.76	C
ATOM	2711	CG	ASN	A	185	8.516	-1.749	30.167	1.00	24.66	C
ATOM	2712	OD1	ASN	A	185	8.523	-2.373	31.230	1.00	23.97	O
ATOM	2713	ND2	ASN	A	185	8.499	-2.338	28.980	1.00	27.88	N
ATOM	2716	C	ASN	A	185	8.548	1.738	31.573	1.00	29.00	C
ATOM	2717	O	ASN	A	185	9.559	2.095	32.225	1.00	29.01	O
ATOM	2718	N	ASN	A	186	7.746	2.594	30.944	1.00	28.56	N
ATOM	2720	CA	ASN	A	186	8.075	4.027	30.880	1.00	29.43	C
ATOM	2722	CB	ASN	A	186	7.331	4.668	29.685	1.00	29.08	C
ATOM	2725	CG	ASN	A	186	7.823	4.171	28.354	1.00	32.85	C
ATOM	2726	OD1	ASN	A	186	7.018	3.960	27.434	1.00	40.10	O
ATOM	2727	ND2	ASN	A	186	9.143	3.982	28.211	1.00	31.78	N
ATOM	2730	C	ASN	A	186	7.794	4.848	32.141	1.00	28.33	C
ATOM	2731	O	ASN	A	186	8.028	6.056	32.153	1.00	29.46	O
ATOM	2732	N	HIS	A	187	7.281	4.258	33.213	1.00	27.62	N
ATOM	2734	CA	HIS	A	187	7.017	4.988	34.436	1.00	26.33	C
ATOM	2736	CB	HIS	A	187	5.532	5.013	34.683	1.00	28.07	C
ATOM	2739	CG	HIS	A	187	4.817	5.971	33.792	1.00	29.28	C
ATOM	2740	ND1	HIS	A	187	4.212	7.111	34.278	1.00	34.07	N
ATOM	2742	CE1	HIS	A	187	3.678	7.779	33.271	1.00	28.09	C
ATOM	2744	NE2	HIS	A	187	3.979	7.155	32.147	1.00	32.42	N
ATOM	2746	CD2	HIS	A	187	4.692	6.016	32.444	1.00	31.59	C
ATOM	2748	C	HIS	A	187	7.789	4.507	35.704	1.00	25.58	C
ATOM	2749	O	HIS	A	187	7.695	5.059	36.790	1.00	24.37	O
ATOM	2750	N	LEU	A	188	8.604	3.488	35.516	1.00	25.54	N
ATOM	2752	CA	LEU	A	188	9.444	3.014	36.624	1.00	24.73	C
ATOM	2754	CB	LEU	A	188	9.856	1.551	36.328	1.00	23.91	C

Figure 5-31

ATOM	2757	CG	LEU	A	188	8.707	0.559	36.298	1.00	25.58	C
ATOM	2759	CD1	LEU	A	188	9.082	-0.800	35.663	1.00	27.12	C
ATOM	2763	CD2	LEU	A	188	8.180	0.346	37.735	1.00	25.35	C
ATOM	2767	C	LEU	A	188	10.691	3.914	36.721	1.00	22.49	C
ATOM	2768	O	LEU	A	188	10.961	4.719	35.853	1.00	21.46	O
ATOM	2769	N	MET	A	189	11.503	3.738	37.747	1.00	22.80	N
ATOM	2771	CA	MET	A	189	12.778	4.485	37.853	1.00	20.65	C
ATOM	2773	CB	MET	A	189	13.411	4.243	39.216	1.00	19.96	C
ATOM	2776	CG	MET	A	189	12.666	4.746	40.414	1.00	23.14	C
ATOM	2779	SE	MET	A	189	13.096	3.964	42.163	1.00	27.61	SE
ATOM	2780	CE	MET	A	189	12.645	5.348	43.227	1.00	30.83	C
ATOM	2784	C	MET	A	189	13.764	4.095	36.785	1.00	19.48	C
ATOM	2785	O	MET	A	189	14.739	4.816	36.543	1.00	19.86	O
ATOM	2786	N	THR	A	190	13.588	2.932	36.183	1.00	18.06	N
ATOM	2788	CA	THR	A	190	14.413	2.468	35.086	1.00	19.60	C
ATOM	2790	CB	THR	A	190	14.526	0.919	35.149	1.00	20.79	C
ATOM	2792	OG1	THR	A	190	13.218	0.402	35.365	1.00	20.11	O
ATOM	2794	CG2	THR	A	190	15.305	0.466	36.402	1.00	19.05	C
ATOM	2798	C	THR	A	190	13.809	2.826	33.724	1.00	19.90	C
ATOM	2799	O	THR	A	190	14.126	2.204	32.729	1.00	18.81	O
ATOM	2800	N	LYS	A	191	12.968	3.854	33.658	1.00	21.69	N
ATOM	2802	CA	LYS	A	191	12.325	4.215	32.365	1.00	22.77	C
ATOM	2804	CB	LYS	A	191	11.402	5.414	32.537	1.00	24.95	C
ATOM	2807	CG	LYS	A	191	12.082	6.640	33.118	1.00	29.61	C
ATOM	2810	CD	LYS	A	191	11.125	7.858	33.298	1.00	35.89	C
ATOM	2813	CE	LYS	A	191	10.000	7.653	34.358	1.00	39.73	C
ATOM	2816	NZ	LYS	A	191	10.373	7.790	35.839	1.00	40.55	N
ATOM	2820	C	LYS	A	191	13.296	4.481	31.236	1.00	22.64	C
ATOM	2821	O	LYS	A	191	12.984	4.273	30.064	1.00	24.95	O
ATOM	2822	N	ASP	A	192	14.489	4.948	31.555	1.00	23.02	N
ATOM	2824	CA	ASP	A	192	15.477	5.287	30.553	1.00	24.11	C
ATOM	2826	CB	ASP	A	192	16.317	6.495	31.058	1.00	25.51	C
ATOM	2829	CG	ASP	A	192	15.505	7.796	31.170	1.00	29.90	C
ATOM	2830	OD1	ASP	A	192	14.490	7.923	30.484	1.00	30.42	O
ATOM	2831	OD2	ASP	A	192	15.802	8.738	31.954	1.00	35.85	O
ATOM	2832	C	ASP	A	192	16.401	4.138	30.157	1.00	22.91	C
ATOM	2833	O	ASP	A	192	17.256	4.301	29.304	1.00	23.13	O
ATOM	2834	N	TYR	A	193	16.254	2.960	30.776	1.00	21.48	N
ATOM	2836	CA	TYR	A	193	17.143	1.852	30.493	1.00	20.18	C
ATOM	2838	CB	TYR	A	193	17.909	1.357	31.802	1.00	21.27	C
ATOM	2841	CG	TYR	A	193	18.276	2.412	32.800	1.00	21.48	C
ATOM	2842	CD1	TYR	A	193	18.965	3.563	32.409	1.00	20.74	C
ATOM	2844	CE1	TYR	A	193	19.306	4.504	33.300	1.00	21.02	C
ATOM	2846	CZ	TYR	A	193	19.015	4.335	34.643	1.00	20.28	C
ATOM	2847	OH	TYR	A	193	19.365	5.347	35.509	1.00	23.63	O
ATOM	2849	CE2	TYR	A	193	18.337	3.216	35.057	1.00	22.33	C
ATOM	2851	CD2	TYR	A	193	17.997	2.253	34.120	1.00	21.41	C
ATOM	2853	C	TYR	A	193	16.406	0.632	29.935	1.00	17.94	C
ATOM	2854	O	TYR	A	193	15.263	0.357	30.266	1.00	20.02	O

Figure 5-32

ATOM	2855	N	PRO	A	194	17.068	-0.151	29.121	1.00	16.91	N
ATOM	2856	CA	PRO	A	194	16.420	-1.366	28.656	1.00	17.28	C
ATOM	2858	CB	PRO	A	194	17.280	-1.800	27.544	1.00	16.33	C
ATOM	2861	CG	PRO	A	194	18.668	-1.253	27.853	1.00	15.86	C
ATOM	2864	CD	PRO	A	194	18.451	-0.027	28.648	1.00	16.65	C
ATOM	2867	C	PRO	A	194	16.459	-2.320	29.810	1.00	16.33	C
ATOM	2868	O	PRO	A	194	17.252	-2.064	30.698	1.00	16.98	O
ATOM	2869	N	ASP	A	195	15.697	-3.383	29.758	1.00	16.36	N
ATOM	2871	CA	ASP	A	195	15.737	-4.405	30.820	1.00	16.37	C
ATOM	2873	CB	ASP	A	195	14.595	-5.385	30.761	1.00	15.91	C
ATOM	2876	CG	ASP	A	195	13.266	-4.768	31.033	1.00	15.16	C
ATOM	2877	OD1	ASP	A	195	13.164	-3.739	31.782	1.00	16.92	O
ATOM	2878	OD2	ASP	A	195	12.211	-5.303	30.564	1.00	18.16	O
ATOM	2879	C	ASP	A	195	17.073	-5.138	30.652	1.00	16.39	C
ATOM	2880	O	ASP	A	195	17.559	-5.407	29.542	1.00	17.26	O
ATOM	2881	N	PRO	A	196	17.688	-5.501	31.748	1.00	14.05	N
ATOM	2882	CA	PRO	A	196	18.979	-6.173	31.636	1.00	14.53	C
ATOM	2884	CB	PRO	A	196	19.467	-6.267	33.115	1.00	14.88	C
ATOM	2887	CG	PRO	A	196	18.249	-6.175	33.945	1.00	15.73	C
ATOM	2890	CD	PRO	A	196	17.229	-5.353	33.132	1.00	15.83	C
ATOM	2893	C	PRO	A	196	18.852	-7.567	31.021	1.00	13.81	C
ATOM	2894	O	PRO	A	196	18.015	-8.430	31.427	1.00	13.69	O
ATOM	2895	N	GLU	A	197	19.702	-7.853	30.057	1.00	14.06	N
ATOM	2897	CA	GLU	A	197	19.695	-9.207	29.555	1.00	13.26	C
ATOM	2899	CB	GLU	A	197	20.611	-9.365	28.356	1.00	15.57	C
ATOM	2902	CG	GLU	A	197	20.210	-8.466	27.161	1.00	16.76	C
ATOM	2905	CD	GLU	A	197	21.015	-7.190	27.070	1.00	17.88	C
ATOM	2906	OE1	GLU	A	197	21.299	-6.447	28.094	1.00	15.83	O
ATOM	2907	OE2	GLU	A	197	21.425	-6.913	25.912	1.00	17.52	O
ATOM	2908	C	GLU	A	197	20.182	-10.192	30.600	1.00	13.28	C
ATOM	2909	O	GLU	A	197	19.830	-11.344	30.536	1.00	12.17	O
ATOM	2910	N	LEU	A	198	21.107	-9.747	31.459	1.00	13.18	N
ATOM	2912	CA	LEU	A	198	21.857	-10.627	32.353	1.00	13.17	C
ATOM	2914	CB	LEU	A	198	23.328	-10.682	31.884	1.00	13.51	C
ATOM	2917	CG	LEU	A	198	24.334	-11.322	32.824	1.00	15.63	C
ATOM	2919	CD1	LEU	A	198	23.976	-12.795	33.038	1.00	13.99	C
ATOM	2923	CD2	LEU	A	198	25.767	-11.149	32.265	1.00	16.77	C
ATOM	2927	C	LEU	A	198	21.827	-10.065	33.767	1.00	13.19	C
ATOM	2928	O	LEU	A	198	22.153	-8.910	33.972	1.00	13.09	O
ATOM	2929	N	LEU	A	199	21.450	-10.920	34.731	1.00	13.10	N
ATOM	2931	CA	LEU	A	199	21.480	-10.554	36.131	1.00	13.29	C
ATOM	2933	CB	LEU	A	199	20.139	-10.863	36.773	1.00	13.24	C
ATOM	2936	CG	LEU	A	199	20.107	-10.650	38.293	1.00	15.28	C
ATOM	2938	CD1	LEU	A	199	20.204	-9.197	38.628	1.00	17.39	C
ATOM	2942	CD2	LEU	A	199	18.809	-11.235	38.815	1.00	18.70	C
ATOM	2946	C	LEU	A	199	22.528	-11.458	36.769	1.00	13.09	C
ATOM	2947	O	LEU	A	199	22.379	-12.706	36.694	1.00	14.10	O
ATOM	2948	N	ILE	A	200	23.578	-10.877	37.345	1.00	13.40	N
ATOM	2950	CA	ILE	A	200	24.536	-11.677	38.119	1.00	13.39	C

Figure 5-33

ATOM	2952	CB	ILE	A	200	25.960	-11.308	37.742	1.00	14.57	C
ATOM	2954	CG1	ILE	A	200	26.242	-11.506	36.253	1.00	15.43	C
ATOM	2957	CD1	ILE	A	200	27.381	-10.652	35.806	1.00	17.40	C
ATOM	2961	CG2	ILE	A	200	26.956	-12.093	38.629	1.00	14.93	C
ATOM	2965	C	ILE	A	200	24.386	-11.417	39.620	1.00	12.73	C
ATOM	2966	O	ILE	A	200	24.362	-10.291	40.071	1.00	13.67	O
ATOM	2967	N	ARG	A	201	24.394	-12.502	40.403	1.00	13.43	N
ATOM	2969	CA	ARG	A	201	24.451	-12.392	41.869	1.00	13.50	C
ATOM	2971	CB	ARG	A	201	23.208	-12.957	42.577	1.00	13.14	C
ATOM	2974	CG	ARG	A	201	23.297	-12.805	44.096	1.00	14.14	C
ATOM	2977	CD	ARG	A	201	22.042	-13.099	44.836	1.00	14.39	C
ATOM	2980	NE	ARG	A	201	22.160	-12.667	46.235	1.00	13.58	N
ATOM	2982	CZ	ARG	A	201	21.144	-12.180	46.941	1.00	15.54	C
ATOM	2983	NH1	ARG	A	201	19.947	-12.067	46.385	1.00	15.76	N
ATOM	2986	NH2	ARG	A	201	21.313	-11.745	48.206	1.00	15.70	N
ATOM	2989	C	ARG	A	201	25.673	-13.181	42.326	1.00	13.59	C
ATOM	2990	O	ARG	A	201	25.803	-14.371	41.967	1.00	15.32	O
ATOM	2991	N	THR	A	202	26.481	-12.545	43.160	1.00	14.91	N
ATOM	2993	CA	THR	A	202	27.678	-13.218	43.706	1.00	15.89	C
ATOM	2995	CB	THR	A	202	28.838	-12.274	43.838	1.00	16.01	C
ATOM	2997	OG1	THR	A	202	28.524	-11.105	44.602	1.00	14.38	O
ATOM	2999	CG2	THR	A	202	29.208	-11.715	42.416	1.00	17.46	C
ATOM	3003	C	THR	A	202	27.390	-13.873	45.048	1.00	16.23	C
ATOM	3004	O	THR	A	202	26.301	-13.660	45.584	1.00	13.87	O
ATOM	3005	N	SER	A	203	28.345	-14.696	45.493	1.00	14.91	N
ATOM	3007	CA	SER	A	203	28.292	-15.429	46.777	1.00	16.85	C
ATOM	3009	CB	SER	A	203	27.642	-14.594	47.903	1.00	16.17	C
ATOM	3012	OG	SER	A	203	26.230	-14.753	48.017	1.00	17.10	O
ATOM	3014	C	SER	A	203	27.691	-16.807	46.778	1.00	17.88	C
ATOM	3015	O	SER	A	203	27.942	-17.573	47.733	1.00	20.07	O
ATOM	3016	N	GLY	A	204	26.885	-17.179	45.767	1.00	17.00	N
ATOM	3018	CA	GLY	A	204	26.231	-18.471	45.733	1.00	17.25	C
ATOM	3021	C	GLY	A	204	24.770	-18.450	46.115	1.00	16.56	C
ATOM	3022	O	GLY	A	204	24.043	-19.443	45.894	1.00	17.87	O
ATOM	3023	N	GLU	A	205	24.294	-17.349	46.691	1.00	14.02	N
ATOM	3025	CA	GLU	A	205	22.888	-17.320	47.067	1.00	15.03	C
ATOM	3027	CB	GLU	A	205	22.558	-16.110	47.913	1.00	15.97	C
ATOM	3030	CG	GLU	A	205	23.376	-16.017	49.197	1.00	16.75	C
ATOM	3033	CD	GLU	A	205	23.247	-17.173	50.177	1.00	22.18	C
ATOM	3034	OE1	GLU	A	205	22.246	-17.892	50.177	1.00	20.42	O
ATOM	3035	OE2	GLU	A	205	24.185	-17.306	51.016	1.00	21.66	O
ATOM	3036	C	GLU	A	205	22.069	-17.296	45.774	1.00	15.08	C
ATOM	3037	O	GLU	A	205	22.508	-16.703	44.769	1.00	14.67	O
ATOM	3038	N	GLN	A	206	20.899	-17.925	45.807	1.00	14.50	N
ATOM	3040	CA	GLN	A	206	20.032	-18.009	44.657	1.00	14.75	C
ATOM	3042	CB	GLN	A	206	19.971	-19.439	44.258	1.00	14.99	C
ATOM	3045	CG	GLN	A	206	21.340	-19.930	43.805	1.00	16.67	C
ATOM	3048	CD	GLN	A	206	21.310	-21.405	43.479	1.00	23.61	C
ATOM	3049	OE1	GLN	A	206	20.894	-21.804	42.392	1.00	27.39	O

Figure 5-34

ATOM	3050	NE2	GLN	A	206	21.710	-22.237	44.468	1.00	31.31	N
ATOM	3053	C	GLN	A	206	18.658	-17.449	44.994	1.00	13.25	C
ATOM	3054	O	GLN	A	206	17.805	-18.167	45.459	1.00	12.74	O
ATOM	3055	N	ARG	A	207	18.533	-16.134	44.811	1.00	12.34	N
ATOM	3057	CA	ARG	A	207	17.334	-15.376	45.123	1.00	12.91	C
ATOM	3059	CB	ARG	A	207	17.091	-15.268	46.624	1.00	12.05	C
ATOM	3062	CG	ARG	A	207	18.290	-15.016	47.403	1.00	15.53	C
ATOM	3065	CD	ARG	A	207	18.028	-15.281	48.895	1.00	15.22	C
ATOM	3068	NE	ARG	A	207	19.049	-14.846	49.836	1.00	16.06	N
ATOM	3070	CZ	ARG	A	207	19.549	-15.596	50.832	1.00	15.70	C
ATOM	3071	NH1	ARG	A	207	19.218	-16.837	50.940	1.00	15.89	N
ATOM	3074	NH2	ARG	A	207	20.449	-15.087	51.684	1.00	17.37	N
ATOM	3077	C	ARG	A	207	17.632	-13.976	44.554	1.00	12.20	C
ATOM	3078	O	ARG	A	207	18.809	-13.590	44.315	1.00	11.73	O
ATOM	3079	N	ILE	A	208	16.555	-13.269	44.283	1.00	11.36	N
ATOM	3081	CA	ILE	A	208	16.671	-11.920	43.729	1.00	13.31	C
ATOM	3083	CB	ILE	A	208	15.722	-11.694	42.556	1.00	13.94	C
ATOM	3085	CG1	ILE	A	208	14.288	-11.641	43.009	1.00	14.75	C
ATOM	3088	CD1	ILE	A	208	13.396	-11.217	41.817	1.00	21.97	C
ATOM	3092	CG2	ILE	A	208	16.027	-12.764	41.467	1.00	18.04	C
ATOM	3096	C	ILE	A	208	16.551	-10.824	44.742	1.00	12.00	C
ATOM	3097	O	ILE	A	208	16.907	-9.667	44.461	1.00	12.69	O
ATOM	3098	N	SER	A	209	16.070	-11.147	45.934	1.00	13.01	N
ATOM	3100	CA	SER	A	209	16.047	-10.185	47.042	1.00	12.86	C
ATOM	3102	CB	SER	A	209	17.439	-10.167	47.755	1.00	12.20	C
ATOM	3105	OG	SER	A	209	17.899	-11.504	48.100	1.00	14.45	O
ATOM	3107	C	SER	A	209	15.504	-8.786	46.664	1.00	13.02	C
ATOM	3108	O	SER	A	209	16.107	-7.728	46.983	1.00	13.38	O
ATOM	3109	N	ASN	A	210	14.327	-8.741	46.020	1.00	13.18	N
ATOM	3111	CA	ASN	A	210	13.675	-7.474	45.701	1.00	13.49	C
ATOM	3113	CB	ASN	A	210	13.416	-6.704	47.017	1.00	14.12	C
ATOM	3116	CG	ASN	A	210	12.223	-5.738	46.956	1.00	15.82	C
ATOM	3117	OD1	ASN	A	210	11.403	-5.787	46.048	1.00	16.94	O
ATOM	3118	ND2	ASN	A	210	12.144	-4.848	47.971	1.00	12.63	N
ATOM	3121	C	ASN	A	210	14.428	-6.608	44.729	1.00	14.07	C
ATOM	3122	O	ASN	A	210	14.185	-5.398	44.642	1.00	15.01	O
ATOM	3123	N	PHE	A	211	15.311	-7.174	43.918	1.00	14.03	N
ATOM	3125	CA	PHE	A	211	16.040	-6.349	42.932	1.00	14.80	C
ATOM	3127	CB	PHE	A	211	17.471	-6.893	42.781	1.00	14.59	C
ATOM	3130	CG	PHE	A	211	18.454	-6.020	42.010	1.00	11.16	C
ATOM	3131	CD1	PHE	A	211	18.671	-4.665	42.313	1.00	15.88	C
ATOM	3133	CE1	PHE	A	211	19.597	-3.919	41.626	1.00	17.55	C
ATOM	3135	CZ	PHE	A	211	20.371	-4.529	40.644	1.00	15.33	C
ATOM	3137	CE2	PHE	A	211	20.198	-5.879	40.360	1.00	14.56	C
ATOM	3139	CD2	PHE	A	211	19.236	-6.599	41.034	1.00	14.74	C
ATOM	3141	C	PHE	A	211	15.412	-6.397	41.530	1.00	15.30	C
ATOM	3142	O	PHE	A	211	15.422	-7.487	40.912	1.00	16.52	O
ATOM	3143	N	LEU	A	212	15.003	-5.245	40.999	1.00	16.59	N
ATOM	3145	CA	LEU	A	212	14.484	-5.135	39.632	1.00	15.65	C

Figure S-35

ATOM	3147	CB	LEU	A	212	15.663	-5.237	38.635	1.00	17.08	C
ATOM	3150	CG	LEU	A	212	16.697	-4.156	38.820	1.00	16.07	C
ATOM	3152	CD1	LEU	A	212	17.887	-4.403	37.950	1.00	16.19	C
ATOM	3156	CD2	LEU	A	212	16.112	-2.740	38.515	1.00	19.75	C
ATOM	3160	C	LEU	A	212	13.463	-6.214	39.339	1.00	16.70	C
ATOM	3161	O	LEU	A	212	13.533	-6.841	38.309	1.00	15.03	O
ATOM	3162	N	ILE	A	213	12.478	-6.400	40.230	1.00	15.76	N
ATOM	3164	CA	ILE	A	213	11.586	-7.569	40.113	1.00	17.00	C
ATOM	3166	CB	ILE	A	213	10.711	-7.746	41.366	1.00	17.75	C
ATOM	3168	CG1	ILE	A	213	9.792	-6.526	41.576	1.00	14.92	C
ATOM	3171	CD1	ILE	A	213	8.999	-6.664	42.810	1.00	18.79	C
ATOM	3175	CG2	ILE	A	213	11.593	-8.034	42.605	1.00	20.78	C
ATOM	3179	C	ILE	A	213	10.750	-7.552	38.820	1.00	16.19	C
ATOM	3180	O	ILE	A	213	10.601	-8.570	38.179	1.00	15.06	O
ATOM	3181	N	TRP	A	214	10.284	-6.380	38.417	1.00	16.99	N
ATOM	3183	CA	TRP	A	214	9.586	-6.244	37.144	1.00	16.50	C
ATOM	3185	CB	TRP	A	214	8.930	-4.879	37.071	1.00	17.50	C
ATOM	3188	CG	TRP	A	214	8.329	-4.527	35.761	1.00	18.05	C
ATOM	3189	CD1	TRP	A	214	8.964	-4.087	34.673	1.00	17.93	C
ATOM	3191	NE1	TRP	A	214	8.069	-3.830	33.661	1.00	17.61	N
ATOM	3193	CE2	TRP	A	214	6.813	-4.115	34.095	1.00	19.39	C
ATOM	3194	CD2	TRP	A	214	6.925	-4.570	35.409	1.00	16.27	C
ATOM	3195	CE3	TRP	A	214	5.780	-4.945	36.074	1.00	18.57	C
ATOM	3197	CZ3	TRP	A	214	4.530	-4.815	35.408	1.00	17.64	C
ATOM	3199	CH2	TRP	A	214	4.478	-4.371	34.098	1.00	18.39	C
ATOM	3201	CZ2	TRP	A	214	5.587	-4.040	33.418	1.00	18.63	C
ATOM	3203	C	TRP	A	214	10.508	-6.383	35.936	1.00	17.21	C
ATOM	3204	O	TRP	A	214	10.211	-7.109	34.983	1.00	16.68	O
ATOM	3205	N	GLN	A	215	11.631	-5.705	36.015	1.00	16.22	N
ATOM	3207	CA	GLN	A	215	12.582	-5.662	34.932	1.00	16.03	C
ATOM	3209	CB	GLN	A	215	13.603	-4.598	35.262	1.00	17.35	C
ATOM	3212	CG	GLN	A	215	13.047	-3.220	35.469	1.00	16.37	C
ATOM	3215	CD	GLN	A	215	12.693	-2.874	36.936	1.00	18.38	C
ATOM	3216	OE1	GLN	A	215	12.564	-3.758	37.761	1.00	16.76	O
ATOM	3217	NE2	GLN	A	215	12.592	-1.542	37.257	1.00	17.18	N
ATOM	3220	C	GLN	A	215	13.307	-7.020	34.588	1.00	15.56	C
ATOM	3221	O	GLN	A	215	13.718	-7.245	33.455	1.00	15.69	O
ATOM	3222	N	VAL	A	216	13.470	-7.933	35.546	1.00	13.88	N
ATOM	3224	CA	VAL	A	216	14.184	-9.175	35.250	1.00	13.69	C
ATOM	3226	CB	VAL	A	216	14.997	-9.717	36.491	1.00	13.05	C
ATOM	3228	CG1	VAL	A	216	16.006	-8.762	36.874	1.00	15.69	C
ATOM	3232	CG2	VAL	A	216	14.033	-10.043	37.613	1.00	17.49	C
ATOM	3236	C	VAL	A	216	13.268	-10.251	34.749	1.00	13.34	C
ATOM	3237	O	VAL	A	216	13.657	-11.404	34.690	1.00	14.39	O
ATOM	3238	N	SER	A	217	12.055	-9.904	34.335	1.00	14.69	N
ATOM	3240	CA	SER	A	217	11.107	-10.874	33.858	1.00	14.90	C
ATOM	3242	CB	SER	A	217	9.939	-10.153	33.165	1.00	16.82	C
ATOM	3245	OG	SER	A	217	8.969	-11.093	32.829	1.00	18.99	O
ATOM	3247	C	SER	A	217	11.667	-11.963	32.931	1.00	14.18	C
ATOM	3248	O	SER	A	217	11.302	-13.143	33.102	1.00	14.20	O

Figure 5-36

ATOM	3249	N	TYR	A	218	12.536	-11.593	31.977	1.00	14.91
ATOM	3251	CA	TYR	A	218	13.160	-12.547	31.068	1.00	15.06
ATOM	3253	CB	TYR	A	218	12.646	-12.376	29.665	1.00	16.66
ATOM	3256	CG	TYR	A	218	11.317	-13.104	29.508	1.00	15.74
ATOM	3257	CD1	TYR	A	218	11.292	-14.468	29.162	1.00	14.99
ATOM	3259	CE1	TYR	A	218	10.117	-15.142	29.034	1.00	16.07
ATOM	3261	CZ	TYR	A	218	8.919	-14.457	29.221	1.00	18.39
ATOM	3262	OH	TYR	A	218	7.714	-15.107	29.094	1.00	18.18
ATOM	3264	CE2	TYR	A	218	8.922	-13.074	29.471	1.00	16.25
ATOM	3266	CD2	TYR	A	218	10.126	-12.430	29.663	1.00	17.49
ATOM	3268	C	TYR	A	218	14.680	-12.462	31.054	1.00	15.62
ATOM	3269	O	TYR	A	218	15.330	-12.958	30.161	1.00	15.35
ATOM	3270	N	SER	A	219	15.232	-11.916	32.127	1.00	13.04
ATOM	3272	CA	SER	A	219	16.645	-11.856	32.257	1.00	13.28
ATOM	3274	CB	SER	A	219	17.035	-10.989	33.457	1.00	11.92
ATOM	3277	OG	SER	A	219	16.617	-9.654	33.427	1.00	12.89
ATOM	3279	C	SER	A	219	17.258	-13.246	32.451	1.00	12.69
ATOM	3280	O	SER	A	219	16.661	-14.118	33.110	1.00	12.81
ATOM	3281	N	GLU	A	220	18.477	-13.441	31.935	1.00	12.84
ATOM	3283	CA	GLU	A	220	19.219	-14.673	32.248	1.00	13.96
ATOM	3285	CB	GLU	A	220	20.346	-14.911	31.216	1.00	13.99
ATOM	3288	CG	GLU	A	220	19.792	-15.371	29.874	1.00	14.97
ATOM	3291	CD	GLU	A	220	19.050	-16.686	29.940	1.00	14.37
ATOM	3292	OE1	GLU	A	220	19.526	-17.668	30.567	1.00	19.15
ATOM	3293	OE2	GLU	A	220	17.935	-16.745	29.418	1.00	16.51
ATOM	3294	C	GLU	A	220	19.859	-14.410	33.602	1.00	13.13
ATOM	3295	O	GLU	A	220	20.357	-13.309	33.829	1.00	15.70
ATOM	3296	N	PHE	A	221	19.897	-15.423	34.458	1.00	13.83
ATOM	3298	CA	PHE	A	221	20.510	-15.342	35.755	1.00	12.76
ATOM	3300	CB	PHE	A	221	19.630	-15.959	36.867	1.00	13.50
ATOM	3303	CG	PHE	A	221	18.255	-15.331	37.073	1.00	14.50
ATOM	3304	CD1	PHE	A	221	17.866	-14.177	36.494	1.00	14.67
ATOM	3306	CE1	PHE	A	221	16.582	-13.632	36.715	1.00	16.57
ATOM	3308	CZ	PHE	A	221	15.774	-14.198	37.563	1.00	19.38
ATOM	3310	CE2	PHE	A	221	16.096	-15.428	38.095	1.00	21.21
ATOM	3312	CD2	PHE	A	221	17.347	-15.965	37.899	1.00	19.71
ATOM	3314	C	PHE	A	221	21.824	-16.194	35.810	1.00	14.83
ATOM	3315	O	PHE	A	221	21.863	-17.384	35.341	1.00	14.56
ATOM	3316	N	ILE	A	222	22.805	-15.612	36.471	1.00	14.76
ATOM	3318	CA	ILE	A	222	24.048	-16.250	36.833	1.00	16.62
ATOM	3320	CB	ILE	A	222	25.230	-15.707	36.052	1.00	16.63
ATOM	3322	CG1	ILE	A	222	25.070	-16.037	34.577	1.00	17.82
ATOM	3325	CD1	ILE	A	222	26.276	-15.557	33.662	1.00	17.73
ATOM	3329	CG2	ILE	A	222	26.547	-16.339	36.621	1.00	20.15
ATOM	3333	C	ILE	A	222	24.291	-16.057	38.344	1.00	15.32
ATOM	3334	O	ILE	A	222	24.409	-14.957	38.872	1.00	15.98
ATOM	3335	N	PHE	A	223	24.359	-17.158	39.028	1.00	16.51
ATOM	3337	CA	PHE	A	223	24.646	-17.128	40.433	1.00	17.44
ATOM	3339	CB	PHE	A	223	23.706	-18.076	41.129	1.00	16.90

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Figure S-37

ATOM	3342	CG	PHE	A	223	22.300	-17.665	40.945	1.00	18.40	C
ATOM	3343	CD1	PHE	A	223	21.859	-16.502	41.537	1.00	21.10	C
ATOM	3345	CE1	PHE	A	223	20.513	-16.015	41.327	1.00	20.44	C
ATOM	3347	CZ	PHE	A	223	19.669	-16.728	40.505	1.00	21.68	C
ATOM	3349	CE2	PHE	A	223	20.111	-17.854	39.886	1.00	23.12	C
ATOM	3351	CD2	PHE	A	223	21.439	-18.327	40.095	1.00	24.21	C
ATOM	3353	C	PHE	A	223	26.108	-17.586	40.541	1.00	17.76	C
ATOM	3354	O	PHE	A	223	26.412	-18.771	40.567	1.00	19.75	O
ATOM	3355	N	ASN	A	224	26.983	-16.588	40.557	1.00	16.51	N
ATOM	3357	CA	ASN	A	224	28.408	-16.752	40.613	1.00	18.01	C
ATOM	3359	CB	ASN	A	224	29.079	-15.484	40.082	1.00	17.90	C
ATOM	3362	CG	ASN	A	224	30.576	-15.605	40.001	1.00	18.91	C
ATOM	3363	OD1	ASN	A	224	31.276	-15.390	40.985	1.00	21.06	O
ATOM	3364	ND2	ASN	A	224	31.089	-15.920	38.808	1.00	22.29	N
ATOM	3367	C	ASN	A	224	28.834	-17.075	42.049	1.00	19.00	C
ATOM	3368	O	ASN	A	224	28.389	-16.431	42.970	1.00	18.26	O
ATOM	3369	N	GLN	A	225	29.698	-18.085	42.247	1.00	20.62	N
ATOM	3371	CA	GLN	A	225	30.075	-18.493	43.613	1.00	22.31	C
ATOM	3373	CB	GLN	A	225	30.629	-19.919	43.629	1.00	23.82	C
ATOM	3376	CG	GLN	A	225	29.742	-21.011	43.090	1.00	26.80	C
ATOM	3379	CD	GLN	A	225	28.453	-21.161	43.818	1.00	29.76	C
ATOM	3380	OE1	GLN	A	225	28.421	-21.479	45.017	1.00	30.57	O
ATOM	3381	NE2	GLN	A	225	27.352	-20.910	43.099	1.00	28.75	N
ATOM	3384	C	GLN	A	225	31.104	-17.624	44.310	1.00	21.73	C
ATOM	3385	O	GLN	A	225	31.271	-17.764	45.520	1.00	22.35	O
ATOM	3386	N	LYS	A	226	31.842	-16.794	43.592	1.00	20.61	N
ATOM	3388	CA	LYS	A	226	32.799	-15.902	44.223	1.00	21.01	C
ATOM	3390	CB	LYS	A	226	33.677	-15.158	43.205	1.00	22.21	C
ATOM	3393	CG	LYS	A	226	34.525	-16.112	42.372	1.00	24.70	C
ATOM	3396	CD	LYS	A	226	35.824	-15.487	41.932	1.00	27.31	C
ATOM	3399	CE	LYS	A	226	36.569	-16.446	41.031	1.00	31.56	C
ATOM	3402	NZ	LYS	A	226	37.751	-15.846	40.365	1.00	34.52	N
ATOM	3406	C	LYS	A	226	32.111	-14.889	45.142	1.00	19.17	C
ATOM	3407	O	LYS	A	226	31.009	-14.449	44.875	1.00	17.51	O
ATOM	3408	N	LEU	A	227	32.737	-14.563	46.257	1.00	16.52	N
ATOM	3410	CA	LEU	A	227	32.253	-13.482	47.087	1.00	17.22	C
ATOM	3412	CB	LEU	A	227	32.954	-13.417	48.461	1.00	17.23	C
ATOM	3415	CG	LEU	A	227	32.658	-14.698	49.224	1.00	16.94	C
ATOM	3417	CD1	LEU	A	227	33.536	-14.737	50.492	1.00	20.33	C
ATOM	3421	CD2	LEU	A	227	31.257	-14.836	49.671	1.00	17.72	C
ATOM	3425	C	LEU	A	227	32.543	-12.216	46.359	1.00	16.55	C
ATOM	3426	O	LEU	A	227	33.529	-12.167	45.643	1.00	17.82	O
ATOM	3427	N	TRP	A	228	31.733	-11.196	46.547	1.00	17.01	N
ATOM	3429	CA	TRP	A	228	31.936	-9.918	45.786	1.00	18.19	C
ATOM	3431	CB	TRP	A	228	30.890	-8.857	46.177	1.00	18.20	C
ATOM	3434	CG	TRP	A	228	31.042	-7.572	45.517	1.00	16.62	C
ATOM	3435	CD1	TRP	A	228	31.364	-6.373	46.087	1.00	18.55	C
ATOM	3437	NE1	TRP	A	228	31.431	-5.402	45.117	1.00	20.27	N
ATOM	3439	CE2	TRP	A	228	31.092	-5.938	43.909	1.00	17.98	C

Figure S-38

ATOM	3440	CD2	TRP	A	228	30.850	-7.299	44.116	1.00	16.76	C
ATOM	3441	CE3	TRP	A	228	30.457	-8.075	43.039	1.00	17.72	C
ATOM	3443	CZ3	TRP	A	228	30.403	-7.498	41.775	1.00	19.09	C
ATOM	3445	CH2	TRP	A	228	30.670	-6.137	41.584	1.00	17.61	C
ATOM	3447	CZ2	TRP	A	228	31.011	-5.329	42.629	1.00	18.27	C
ATOM	3449	C	TRP	A	228	33.393	-9.342	45.799	1.00	20.13	C
ATOM	3450	O	TRP	A	228	33.894	-9.009	44.714	1.00	19.19	O
ATOM	3451	N	PRO	A	229	34.066	-9.172	46.964	1.00	20.92	N
ATOM	3452	CA	PRO	A	229	35.435	-8.627	46.961	1.00	21.88	C
ATOM	3454	CB	PRO	A	229	35.783	-8.555	48.456	1.00	22.44	C
ATOM	3457	CG	PRO	A	229	34.449	-8.494	49.142	1.00	23.36	C
ATOM	3460	CD	PRO	A	229	33.601	-9.413	48.332	1.00	20.09	C
ATOM	3463	C	PRO	A	229	36.432	-9.482	46.148	1.00	21.54	C
ATOM	3464	O	PRO	A	229	37.523	-8.977	45.803	1.00	23.91	O
ATOM	3465	N	ASP	A	230	36.072	-10.718	45.796	1.00	20.21	N
ATOM	3467	CA	ASP	A	230	36.931	-11.565	44.987	1.00	20.59	C
ATOM	3469	CB	ASP	A	230	36.895	-13.042	45.451	1.00	19.78	C
ATOM	3472	CG	ASP	A	230	37.447	-13.239	46.852	1.00	21.05	C
ATOM	3473	OD1	ASP	A	230	38.441	-12.594	47.154	1.00	21.15	O
ATOM	3474	OD2	ASP	A	230	36.917	-13.984	47.698	1.00	20.21	O
ATOM	3475	C	ASP	A	230	36.517	-11.529	43.522	1.00	20.75	C
ATOM	3476	O	ASP	A	230	37.176	-12.144	42.659	1.00	21.42	O
ATOM	3477	N	PHE	A	231	35.384	-10.874	43.237	1.00	19.89	N
ATOM	3479	CA	PHE	A	231	34.868	-10.794	41.870	1.00	20.25	C
ATOM	3481	CB	PHE	A	231	33.406	-10.376	41.890	1.00	18.89	C
ATOM	3484	CG	PHE	A	231	32.652	-10.598	40.584	1.00	17.28	C
ATOM	3485	CD1	PHE	A	231	32.401	-9.542	39.722	1.00	18.12	C
ATOM	3487	CE1	PHE	A	231	31.708	-9.749	38.569	1.00	18.75	C
ATOM	3489	CZ	PHE	A	231	31.200	-11.024	38.248	1.00	16.55	C
ATOM	3491	CE2	PHE	A	231	31.444	-12.063	39.082	1.00	20.51	C
ATOM	3493	CD2	PHE	A	231	32.154	-11.844	40.254	1.00	18.64	C
ATOM	3495	C	PHE	A	231	35.754	-9.796	41.135	1.00	21.09	C
ATOM	3496	O	PHE	A	231	36.143	-8.774	41.687	1.00	24.24	O
ATOM	3497	N	ASP	A	232	36.197	-10.185	39.943	1.00	23.02	N
ATOM	3499	CA	ASP	A	232	37.131	-9.376	39.190	1.00	24.11	C
ATOM	3501	CB	ASP	A	232	38.598	-9.845	39.413	1.00	24.14	C
ATOM	3504	CG	ASP	A	232	38.874	-11.249	38.963	1.00	25.04	C
ATOM	3505	OD1	ASP	A	232	38.135	-11.855	38.160	1.00	21.94	O
ATOM	3506	OD2	ASP	A	232	39.896	-11.872	39.359	1.00	30.24	O
ATOM	3507	C	ASP	A	232	36.803	-9.303	37.696	1.00	25.60	C
ATOM	3508	O	ASP	A	232	35.825	-9.904	37.223	1.00	24.87	O
ATOM	3509	N	GLU	A	233	37.647	-8.588	36.970	1.00	25.37	N
ATOM	3511	CA	GLU	A	233	37.460	-8.422	35.515	1.00	26.59	C
ATOM	3513	CB	GLU	A	233	38.650	-7.680	34.920	1.00	27.13	C
ATOM	3516	CG	GLU	A	233	38.688	-6.226	35.365	1.00	30.62	C
ATOM	3519	CD	GLU	A	233	39.654	-5.942	36.510	1.00	33.39	C
ATOM	3520	OE1	GLU	A	233	39.794	-6.798	37.422	1.00	33.08	O
ATOM	3521	OE2	GLU	A	233	40.219	-4.835	36.491	1.00	28.43	O
ATOM	3522	C	GLU	A	233	37.285	-9.755	34.833	1.00	25.04	C

Figure S-39

ATOM	3523	O	GLU	A	233	36.360	-9.958	34.047	1.00	24.40	O
ATOM	3524	N	ASP	A	234	38.153	-10.703	35.146	1.00	25.47	N
ATOM	3526	CA	ASP	A	234	38.086	-11.996	34.518	1.00	24.83	C
ATOM	3528	CB	ASP	A	234	39.348	-12.821	34.776	1.00	27.09	C
ATOM	3531	CG	ASP	A	234	40.580	-12.251	34.016	1.00	29.02	C
ATOM	3532	OD1	ASP	A	234	40.440	-11.758	32.891	1.00	38.07	O
ATOM	3533	OD2	ASP	A	234	41.724	-12.209	34.464	1.00	34.87	O
ATOM	3534	C	ASP	A	234	36.808	-12.782	34.811	1.00	24.62	C
ATOM	3535	O	ASP	A	234	36.261	-13.470	33.897	1.00	22.52	O
ATOM	3536	N	GLU	A	235	36.342	-12.720	36.070	1.00	22.13	N
ATOM	3538	CA	GLU	A	235	35.082	-13.355	36.429	1.00	21.63	C
ATOM	3540	CB	GLU	A	235	34.806	-13.251	37.946	1.00	20.42	C
ATOM	3543	CG	GLU	A	235	33.907	-14.363	38.450	1.00	18.84	C
ATOM	3546	CD	GLU	A	235	34.498	-15.749	38.323	1.00	22.29	C
ATOM	3547	OE1	GLU	A	235	35.741	-15.857	38.140	1.00	24.43	O
ATOM	3548	OE2	GLU	A	235	33.741	-16.724	38.344	1.00	21.68	O
ATOM	3549	C	GLU	A	235	33.896	-12.770	35.611	1.00	19.41	C
ATOM	3550	O	GLU	A	235	33.023	-13.509	35.182	1.00	20.14	O
ATOM	3551	N	LEU	A	236	33.853	-11.453	35.422	1.00	19.36	N
ATOM	3553	CA	LEU	A	236	32.819	-10.831	34.628	1.00	20.06	C
ATOM	3555	CB	LEU	A	236	32.917	-9.337	34.637	1.00	20.11	C
ATOM	3558	CG	LEU	A	236	31.814	-8.667	33.805	1.00	23.04	C
ATOM	3560	CD1	LEU	A	236	30.487	-8.833	34.495	1.00	20.12	C
ATOM	3564	CD2	LEU	A	236	32.127	-7.196	33.545	1.00	24.97	C
ATOM	3568	C	LEU	A	236	32.811	-11.342	33.161	1.00	20.82	C
ATOM	3569	O	LEU	A	236	31.779	-11.673	32.607	1.00	19.88	O
ATOM	3570	N	ILE	A	237	33.991	-11.439	32.570	1.00	20.29	N
ATOM	3572	CA	ILE	A	237	34.088	-11.984	31.241	1.00	20.52	C
ATOM	3574	CB	ILE	A	237	35.535	-11.869	30.736	1.00	20.17	C
ATOM	3576	CG1	ILE	A	237	35.973	-10.437	30.725	1.00	21.96	C
ATOM	3579	CD1	ILE	A	237	35.284	-9.549	29.781	1.00	23.17	C
ATOM	3583	CG2	ILE	A	237	35.687	-12.516	29.372	1.00	20.41	C
ATOM	3587	C	ILE	A	237	33.623	-13.408	31.195	1.00	19.83	C
ATOM	3588	O	ILE	A	237	32.954	-13.805	30.272	1.00	21.67	O
ATOM	3589	N	LYS	A	238	33.982	-14.228	32.170	1.00	21.01	N
ATOM	3591	CA	LYS	A	238	33.475	-15.591	32.196	1.00	20.77	C
ATOM	3593	CB	LYS	A	238	34.033	-16.351	33.387	1.00	22.98	C
ATOM	3596	CG	LYS	A	238	35.567	-16.387	33.418	1.00	29.03	C
ATOM	3599	CD	LYS	A	238	36.167	-16.630	34.836	1.00	35.34	C
ATOM	3602	CE	LYS	A	238	35.878	-18.005	35.408	1.00	36.70	C
ATOM	3605	NZ	LYS	A	238	36.506	-18.218	36.817	1.00	38.95	N
ATOM	3609	C	LYS	A	238	31.927	-15.620	32.305	1.00	19.64	C
ATOM	3610	O	LYS	A	238	31.258	-16.464	31.738	1.00	19.66	O
ATOM	3611	N	CYS	A	239	31.377	-14.693	33.077	1.00	19.50	N
ATOM	3613	CA	CYS	A	239	29.928	-14.593	33.176	1.00	19.36	C
ATOM	3615	CB	CYS	A	239	29.598	-13.528	34.228	1.00	19.01	C
ATOM	3618	SG	CYS	A	239	29.835	-14.128	35.949	1.00	21.25	S
ATOM	3619	C	CYS	A	239	29.291	-14.217	31.828	1.00	18.46	C
ATOM	3620	O	CYS	A	239	28.247	-14.736	31.441	1.00	18.38	O

Figure S-40

ATOM	3621	N	ILE	A	240	29.887	-13.262	31.148	1.00	19.63	N
ATOM	3623	CA	ILE	A	240	29.365	-12.845	29.834	1.00	19.74	C
ATOM	3625	CB	ILE	A	240	30.101	-11.645	29.321	1.00	19.44	C
ATOM	3627	CG1	ILE	A	240	29.815	-10.456	30.214	1.00	21.51	C
ATOM	3630	CD1	ILE	A	240	30.478	-9.212	29.810	1.00	23.28	C
ATOM	3634	CG2	ILE	A	240	29.715	-11.314	27.930	1.00	20.44	C
ATOM	3638	C	ILE	A	240	29.420	-14.010	28.851	1.00	20.46	C
ATOM	3639	O	ILE	A	240	28.477	-14.225	28.090	1.00	18.92	O
ATOM	3640	N	LYS	A	241	30.499	-14.787	28.925	1.00	20.23	N
ATOM	3642	CA	LYS	A	241	30.663	-15.981	28.094	1.00	21.54	C
ATOM	3644	CB	LYS	A	241	32.031	-16.621	28.344	1.00	23.92	C
ATOM	3647	CG	LYS	A	241	32.442	-17.723	27.364	1.00	29.41	C
ATOM	3650	CD	LYS	A	241	33.959	-18.098	27.572	1.00	35.42	C
ATOM	3653	CE	LYS	A	241	34.960	-17.003	27.139	1.00	39.23	C
ATOM	3656	NZ	LYS	A	241	36.429	-17.318	27.559	1.00	43.58	N
ATOM	3660	C	LYS	A	241	29.579	-16.966	28.377	1.00	21.27	C
ATOM	3661	O	LYS	A	241	28.963	-17.526	27.453	1.00	19.09	O
ATOM	3662	N	ILE	A	242	29.283	-17.175	29.660	1.00	20.22	N
ATOM	3664	CA	ILE	A	242	28.223	-18.111	30.014	1.00	19.74	C
ATOM	3666	CB	ILE	A	242	28.101	-18.293	31.538	1.00	20.05	C
ATOM	3668	CG1	ILE	A	242	29.242	-19.141	32.053	1.00	21.50	C
ATOM	3671	CD1	ILE	A	242	29.358	-19.214	33.562	1.00	21.34	C
ATOM	3675	CG2	ILE	A	242	26.704	-18.847	31.887	1.00	19.73	C
ATOM	3679	C	ILE	A	242	26.924	-17.550	29.443	1.00	18.93	C
ATOM	3680	O	ILE	A	242	26.120	-18.270	28.859	1.00	18.46	O
ATOM	3681	N	TYR	A	243	26.697	-16.247	29.635	1.00	17.59	N
ATOM	3683	CA	TYR	A	243	25.506	-15.626	29.097	1.00	17.03	C
ATOM	3685	CB	TYR	A	243	25.515	-14.107	29.393	1.00	18.54	C
ATOM	3688	CG	TYR	A	243	24.487	-13.382	28.540	1.00	16.47	C
ATOM	3689	CD1	TYR	A	243	23.128	-13.435	28.853	1.00	14.87	C
ATOM	3691	CE1	TYR	A	243	22.154	-12.786	28.060	1.00	14.43	C
ATOM	3693	CZ	TYR	A	243	22.545	-12.140	26.931	1.00	18.52	C
ATOM	3694	OH	TYR	A	243	21.584	-11.601	26.142	1.00	15.59	O
ATOM	3696	CE2	TYR	A	243	23.875	-12.120	26.557	1.00	17.47	C
ATOM	3698	CD2	TYR	A	243	24.851	-12.721	27.382	1.00	18.49	C
ATOM	3700	C	TYR	A	243	25.306	-15.899	27.580	1.00	17.74	C
ATOM	3701	O	TYR	A	243	24.198	-16.238	27.103	1.00	16.28	O
ATOM	3702	N	GLN	A	244	26.376	-15.770	26.815	1.00	18.16	N
ATOM	3704	CA	GLN	A	244	26.285	-15.914	25.360	1.00	18.81	C
ATOM	3706	CB	GLN	A	244	27.621	-15.427	24.714	1.00	18.50	C
ATOM	3709	CG	GLN	A	244	27.791	-13.865	24.815	1.00	17.89	C
ATOM	3712	CD	GLN	A	244	29.053	-13.324	24.121	1.00	19.24	C
ATOM	3713	OE1	GLN	A	244	29.156	-12.139	23.806	1.00	22.54	O
ATOM	3714	NE2	GLN	A	244	30.008	-14.178	23.934	1.00	22.15	N
ATOM	3717	C	GLN	A	244	25.872	-17.302	24.915	1.00	20.22	C
ATOM	3718	O	GLN	A	244	25.436	-17.510	23.768	1.00	21.47	O
ATOM	3719	N	SER	A	245	26.040	-18.273	25.794	1.00	19.88	N
ATOM	3721	CA	SER	A	245	25.692	-19.630	25.518	1.00	21.03	C
ATOM	3723	CB	SER	A	245	26.577	-20.531	26.343	1.00	23.16	C

Figure S-41

ATOM	3726	OG	SER	A	245	26.150	-20.564	27.745	1.00	28.07	O
ATOM	3728	C	SER	A	245	24.251	-19.943	25.853	1.00	21.10	C
ATOM	3729	O	SER	A	245	23.754	-21.017	25.521	1.00	19.69	O
ATOM	3730	N	ARG	A	246	23.594	-19.044	26.589	1.00	19.29	N
ATOM	3732	CA	ARG	A	246	22.207	-19.308	26.944	1.00	18.84	C
ATOM	3734	CB	ARG	A	246	21.771	-18.321	27.998	1.00	20.45	C
ATOM	3737	CG	ARG	A	246	22.576	-18.384	29.256	1.00	17.50	C
ATOM	3740	CD	ARG	A	246	22.226	-19.593	30.108	1.00	19.65	C
ATOM	3743	NE	ARG	A	246	22.959	-19.651	31.371	1.00	18.24	N
ATOM	3745	CZ	ARG	A	246	22.573	-19.030	32.488	1.00	18.27	C
ATOM	3746	NH1	ARG	A	246	21.503	-18.262	32.496	1.00	15.88	N
ATOM	3749	NH2	ARG	A	246	23.271	-19.167	33.608	1.00	17.71	N
ATOM	3752	C	ARG	A	246	21.296	-19.200	25.728	1.00	20.45	C
ATOM	3753	O	ARG	A	246	21.556	-18.385	24.852	1.00	20.25	O
ATOM	3754	N	GLN	A	247	20.243	-20.011	25.671	1.00	19.33	N
ATOM	3756	CA	GLN	A	247	19.293	-20.002	24.569	1.00	19.81	C
ATOM	3758	CB	GLN	A	247	19.007	-21.468	24.167	1.00	20.03	C
ATOM	3761	CG	GLN	A	247	20.292	-22.247	23.814	1.00	25.50	C
ATOM	3764	CD	GLN	A	247	20.934	-21.738	22.535	1.00	34.35	C
ATOM	3765	OE1	GLN	A	247	22.145	-21.387	22.508	1.00	38.94	O
ATOM	3766	NE2	GLN	A	247	20.134	-21.677	21.471	1.00	32.88	N
ATOM	3769	C	GLN	A	247	18.040	-19.269	25.030	1.00	18.59	C
ATOM	3770	O	GLN	A	247	17.243	-19.821	25.785	1.00	18.17	O
ATOM	3771	N	ARG	A	248	17.871	-18.008	24.618	1.00	15.34	N
ATOM	3773	CA	ARG	A	248	16.759	-17.219	25.106	1.00	16.50	C
ATOM	3775	CB	ARG	A	248	17.151	-15.758	25.124	1.00	17.26	C
ATOM	3778	CG	ARG	A	248	18.500	-15.510	25.856	1.00	18.94	C
ATOM	3781	CD	ARG	A	248	18.840	-14.053	25.911	1.00	20.88	C
ATOM	3784	NE	ARG	A	248	17.970	-13.462	26.907	1.00	23.36	N
ATOM	3786	CZ	ARG	A	248	17.708	-12.156	27.027	1.00	28.62	C
ATOM	3787	NH1	ARG	A	248	18.165	-11.272	26.134	1.00	22.79	N
ATOM	3790	NH2	ARG	A	248	16.913	-11.747	28.009	1.00	27.91	N
ATOM	3793	C	ARG	A	248	15.546	-17.443	24.201	1.00	17.65	C
ATOM	3794	O	ARG	A	248	15.691	-17.381	22.958	1.00	17.79	O
ATOM	3795	N	ARG	A	249	14.386	-17.651	24.798	1.00	17.10	N
ATOM	3797	CA	ARG	A	249	13.160	-17.962	24.041	1.00	17.98	C
ATOM	3799	CB	ARG	A	249	12.733	-19.398	24.301	1.00	18.16	C
ATOM	3802	CG	ARG	A	249	13.777	-20.387	23.745	1.00	19.25	C
ATOM	3805	CD	ARG	A	249	13.394	-21.836	23.806	1.00	21.98	C
ATOM	3808	NE	ARG	A	249	13.646	-22.456	25.103	1.00	27.22	N
ATOM	3810	CZ	ARG	A	249	14.793	-23.012	25.447	1.00	27.68	C
ATOM	3811	NH1	ARG	A	249	15.815	-23.005	24.604	1.00	27.19	N
ATOM	3814	NH2	ARG	A	249	14.898	-23.591	26.632	1.00	29.40	N
ATOM	3817	C	ARG	A	249	11.971	-17.051	24.173	1.00	18.34	C
ATOM	3818	O	ARG	A	249	11.119	-17.011	23.265	1.00	16.92	O
ATOM	3819	N	PHE	A	250	11.864	-16.342	25.297	1.00	18.11	N
ATOM	3821	CA	PHE	A	250	10.798	-15.366	25.521	1.00	18.50	C
ATOM	3823	CB	PHE	A	250	11.010	-14.149	24.593	1.00	18.85	C
ATOM	3826	CG	PHE	A	250	12.406	-13.613	24.653	1.00	21.51	C
ATOM	3827	CD1	PHE	A	250	12.819	-12.853	25.744	1.00	20.03	C
ATOM	3829	CE1	PHE	A	250	14.157	-12.402	25.820	1.00	24.51	C
ATOM	3831	CZ	PHE	A	250	15.046	-12.731	24.854	1.00	24.30	C

Figure S-42

ATOM	3833	CE2	PHE	A	250	14.654	-13.495	23.774	1.00	25.65	C
ATOM	3835	CD2	PHE	A	250	13.339	-13.958	23.695	1.00	25.24	C
ATOM	3837	C	PHE	A	250	9.393	-15.962	25.375	1.00	18.97	C
ATOM	3838	O	PHE	A	250	8.475	-15.296	24.896	1.00	19.60	O
ATOM	3839	N	GLY	A	251	9.233	-17.243	25.737	1.00	18.74	N
ATOM	3841	CA	GLY	A	251	7.952	-17.883	25.707	1.00	17.68	C
ATOM	3844	C	GLY	A	251	7.678	-18.671	24.427	1.00	19.01	C
ATOM	3845	O	GLY	A	251	6.716	-19.437	24.396	1.00	17.74	O
ATOM	3846	N	GLY	A	252	8.559	-18.521	23.444	1.00	20.08	N
ATOM	3848	CA	GLY	A	252	8.400	-19.146	22.132	1.00	20.97	C
ATOM	3851	C	GLY	A	252	9.316	-20.333	22.019	1.00	21.61	C
ATOM	3852	O	GLY	A	252	9.794	-20.875	23.025	1.00	19.17	O
ATOM	3853	N	LEU	A	253	9.562	-20.762	20.784	1.00	20.83	N
ATOM	3855	CA	LEU	A	253	10.398	-21.911	20.560	1.00	21.55	C
ATOM	3857	CB	LEU	A	253	9.757	-22.951	19.605	1.00	20.69	C
ATOM	3860	CG	LEU	A	253	8.343	-23.447	19.891	1.00	22.26	C
ATOM	3862	CD1	LEU	A	253	7.998	-24.557	18.900	1.00	24.29	C
ATOM	3866	CD2	LEU	A	253	8.173	-23.977	21.364	1.00	19.64	C
ATOM	3870	C	LEU	A	253	11.710	-21.423	19.996	1.00	24.06	C
ATOM	3871	O	LEU	A	253	11.804	-20.355	19.424	1.00	25.75	O
ATOM	3872	N	SER	A	254	12.735	-22.196	20.224	1.00	27.07	N
ATOM	3874	CA	SER	A	254	14.054	-21.935	19.674	1.00	29.97	C
ATOM	3876	CB	SER	A	254	15.112	-22.715	20.463	1.00	30.67	C
ATOM	3879	OG	SER	A	254	15.578	-22.007	21.640	1.00	30.26	O
ATOM	3881	C	SER	A	254	13.971	-22.452	18.236	1.00	32.30	C
ATOM	3882	O	SER	A	254	13.092	-23.258	17.912	1.00	31.98	O
ATOM	3883	N	GLU	A	255	14.874	-21.990	17.376	1.00	35.30	N
ATOM	3885	CA	GLU	A	255	14.856	-22.383	15.964	1.00	37.74	C
ATOM	3887	CB	GLU	A	255	15.932	-21.594	15.185	1.00	38.66	C
ATOM	3890	CG	GLU	A	255	15.820	-20.090	15.425	1.00	41.46	C
ATOM	3893	CD	GLU	A	255	16.325	-19.210	14.286	1.00	47.45	C
ATOM	3894	OE1	GLU	A	255	16.885	-19.726	13.284	1.00	52.64	O
ATOM	3895	OE2	GLU	A	255	16.168	-17.975	14.400	1.00	50.98	O
ATOM	3896	C	GLU	A	255	15.005	-23.902	15.778	1.00	38.42	C
ATOM	3897	O	GLU	A	255	15.579	-24.600	16.624	1.00	37.87	O
ATOM	3898	N	GLU	A	256	14.451	-24.448	14.693	1.00	39.64	N
ATOM	3900	CA	GLU	A	256	14.648	-25.883	14.473	1.00	40.53	C
ATOM	3902	CB	GLU	A	256	13.723	-26.452	13.380	1.00	40.46	C
ATOM	3905	CG	GLU	A	256	12.270	-26.596	13.864	1.00	41.03	C
ATOM	3908	CD	GLU	A	256	11.997	-27.895	14.620	1.00	41.28	C
ATOM	3909	OE1	GLU	A	256	12.950	-28.652	14.918	1.00	39.86	O
ATOM	3910	OE2	GLU	A	256	10.824	-28.153	14.934	1.00	40.76	O
ATOM	3911	C	GLU	A	256	16.143	-26.127	14.168	1.00	41.41	C
ATOM	3912	O	GLU	A	256	16.750	-27.060	14.733	1.00	43.09	O
ATOM	3913	OXT	GLU	A	256	16.785	-25.413	13.396	1.00	39.80	O
ATOM	3914	MG	MG	M	1	24.402	-10.895	51.726	1.00	17.72	MG
ATOM	3915	S	SO4	S	901	19.470	-11.342	51.217	1.00	18.01	S
ATOM	3916	O1	SO4	S	901	19.973	-10.251	50.420	1.00	16.95	O
ATOM	3917	O2	SO4	S	901	18.379	-12.038	50.587	1.00	16.47	O

Figure S-43

ATOM	3918	O3	SO4	S	901	18.991	-10.911	52.570	1.00	17.36	O
ATOM	3919	O4	SO4	S	901	20.548	-12.266	51.441	1.00	19.77	O
ATOM	3920	O1B	FPP	F	999	28.376	-12.033	53.033	1.00	19.79	O
ATOM	3921	PB	FPP	F	999	27.113	-11.258	53.233	1.00	21.01	P
ATOM	3922	O2B	FPP	F	999	25.882	-11.938	52.655	1.00	23.30	O
ATOM	3924	O3B	FPP	F	999	26.872	-10.808	54.632	1.00	24.58	O
ATOM	3926	O3A	FPP	F	999	27.401	-9.878	52.532	1.00	19.69	O
ATOM	3927	PA	FPP	F	999	26.569	-8.650	52.316	1.00	20.20	P
ATOM	3928	O1A	FPP	F	999	26.865	-7.561	53.347	1.00	18.02	O
ATOM	3929	O2A	FPP	F	999	25.087	-9.038	52.264	1.00	15.47	O
ATOM	3931	O1	FPP	F	999	26.996	-8.086	50.939	1.00	19.51	O
ATOM	3932	C1	FPP	F	999	26.190	-7.124	50.209	1.00	23.76	C
ATOM	3935	C2	FPP	F	999	26.789	-5.771	49.974	1.00	27.70	C
ATOM	3937	C3	FPP	F	999	26.041	-4.697	49.771	1.00	34.57	C
ATOM	3938	C4	FPP	F	999	24.546	-4.813	49.692	1.00	39.88	C
ATOM	3942	C5	FPP	F	999	26.518	-3.274	49.546	1.00	38.78	C
ATOM	3945	C6	FPP	F	999	27.888	-2.810	49.919	1.00	37.03	C
ATOM	3948	C7	FPP	F	999	27.806	-1.544	49.114	1.00	36.76	C
ATOM	3950	C8	FPP	F	999	28.808	-0.756	48.788	1.00	40.82	C
ATOM	3951	C10	FPP	F	999	30.198	-1.044	49.268	1.00	42.60	C
ATOM	3955	C9	FPP	F	999	28.382	0.410	47.930	1.00	42.71	C
ATOM	3958	C11	FPP	F	999	29.208	1.658	47.877	1.00	44.36	C
ATOM	3961	C12	FPP	F	999	28.296	2.686	47.229	1.00	45.96	C
ATOM	3963	C13	FPP	F	999	28.669	3.466	46.212	1.00	47.78	C
ATOM	3964	C15	FPP	F	999	29.931	3.291	45.446	1.00	46.95	C
ATOM	3968	C14	FPP	F	999	27.770	4.582	45.770	1.00	49.85	C
ATOM	3972	O	HOH	Y	1	23.313	-11.049	53.402	1.00	20.47	O
ATOM	3973	O	HOH	Y	2	23.250	-12.575	51.192	1.00	21.44	O
ATOM	3974	O	HOH	Y	3	20.827	-9.512	53.986	1.00	17.71	O
ATOM	3975	O	HOH	Y	4	22.702	-9.879	50.685	1.00	18.03	O
ATOM	3976	O	HOH	W	1	13.554	-9.050	31.328	1.00	16.05	O
ATOM	3979	O	HOH	W	2	18.797	-20.238	31.134	1.00	15.63	O
ATOM	3982	O	HOH	W	3	10.787	-3.727	40.028	1.00	19.33	O
ATOM	3985	O	HOH	W	4	16.866	-13.710	52.157	1.00	15.96	O
ATOM	3988	O	HOH	W	5	7.680	-9.956	30.645	1.00	21.10	O
ATOM	3991	O	HOH	W	6	15.854	-9.310	29.847	1.00	18.77	O
ATOM	3994	O	HOH	W	7	14.610	-1.450	32.566	1.00	19.52	O
ATOM	3997	O	HOH	W	8	20.632	-8.068	23.642	1.00	21.10	O
ATOM	4000	O	HOH	W	9	12.112	-7.678	29.443	1.00	22.56	O
ATOM	4003	O	HOH	W	10	20.061	-7.807	50.674	1.00	20.15	O
ATOM	4006	O	HOH	W	11	25.142	-16.426	43.634	1.00	17.77	O
ATOM	4009	O	HOH	W	12	29.663	-18.260	37.334	1.00	21.64	O
ATOM	4012	O	HOH	W	13	24.691	-2.457	21.480	1.00	20.52	O
ATOM	4015	O	HOH	W	14	20.052	9.325	38.406	1.00	24.32	O
ATOM	4018	O	HOH	W	15	31.285	-3.416	22.253	1.00	27.18	O
ATOM	4021	O	HOH	W	16	15.623	5.663	33.972	1.00	22.83	O

Figure 5-44

ATOM	4024	O	HOH	W	17	29.817	1.759	27.213	1.00	23.21	O
ATOM	4027	O	HOH	W	18	25.598	-21.416	34.586	1.00	32.69	O
ATOM	4030	O	HOH	W	19	37.814	-14.883	50.040	1.00	22.89	O
ATOM	4033	O	HOH	W	20	25.835	3.937	27.521	1.00	20.57	O
ATOM	4036	O	HOH	W	21	30.573	-16.932	23.338	1.00	24.29	O
ATOM	4039	O	HOH	W	22	19.015	-4.622	25.220	1.00	22.62	O
ATOM	4042	O	HOH	W	23	30.724	-19.405	39.910	1.00	24.66	O
ATOM	4045	O	HOH	W	24	32.257	1.783	25.995	1.00	24.75	O
ATOM	4048	O	HOH	W	25	35.164	-15.904	46.795	1.00	22.69	O
ATOM	4051	O	HOH	W	26	32.317	-5.326	20.719	1.00	24.73	O
ATOM	4054	O	HOH	W	27	11.042	-2.349	32.597	1.00	21.09	O
ATOM	4057	O	HOH	W	28	11.617	0.284	32.894	1.00	21.57	O
ATOM	4060	O	HOH	W	29	21.898	-19.939	51.879	1.00	21.55	O
ATOM	4063	O	HOH	W	30	14.058	-14.169	34.194	1.00	17.95	O
ATOM	4066	O	HOH	W	31	15.917	-15.155	28.554	1.00	17.04	O
ATOM	4069	O	HOH	W	32	2.475	-10.516	31.120	1.00	18.73	O
ATOM	4072	O	HOH	W	33	26.062	7.943	28.903	1.00	25.77	O
ATOM	4075	O	HOH	W	34	-0.543	-7.027	30.010	1.00	31.49	O
ATOM	4078	O	HOH	W	35	12.149	-24.737	21.402	1.00	26.93	O
ATOM	4081	O	HOH	W	36	23.820	1.896	21.363	1.00	26.86	O
ATOM	4084	O	HOH	W	37	19.836	-24.443	41.962	1.00	18.28	O
ATOM	4087	O	HOH	W	38	32.644	-16.354	56.029	1.00	28.72	O
ATOM	4090	O	HOH	W	39	26.212	-3.793	23.123	1.00	22.27	O
ATOM	4093	O	HOH	W	40	32.366	4.468	29.120	1.00	26.39	O
ATOM	4096	O	HOH	W	41	29.971	-3.791	47.450	1.00	30.40	O
ATOM	4099	O	HOH	W	42	19.104	-11.893	23.940	1.00	25.36	O
ATOM	4102	O	HOH	W	43	18.193	7.384	37.013	1.00	31.69	O
ATOM	4105	O	HOH	W	44	35.950	-0.047	24.188	1.00	27.81	O
ATOM	4108	O	HOH	W	45	40.392	8.489	39.399	1.00	30.80	O
ATOM	4111	O	HOH	W	46	28.385	4.369	63.297	1.00	30.77	O
ATOM	4114	O	HOH	W	47	29.114	-3.307	61.510	1.00	31.70	O
ATOM	4117	O	HOH	W	48	19.531	-17.084	22.607	1.00	22.10	O
ATOM	4120	O	HOH	W	49	17.604	7.911	42.347	1.00	32.51	O
ATOM	4123	O	HOH	W	50	20.055	-4.772	63.588	1.00	29.92	O
ATOM	4126	O	HOH	W	51	24.808	11.941	35.425	1.00	23.22	O
ATOM	4129	O	HOH	W	52	9.660	-8.982	28.818	1.00	32.56	O
ATOM	4132	O	HOH	W	53	23.677	5.214	26.599	1.00	24.47	O
ATOM	4135	O	HOH	W	54	16.457	-2.305	34.563	1.00	22.90	O
ATOM	4138	O	HOH	W	55	22.364	-10.524	23.927	1.00	25.15	O
ATOM	4141	O	HOH	W	56	24.819	-21.382	44.230	1.00	28.57	O
ATOM	4144	O	HOH	W	57	15.440	6.944	40.805	1.00	30.44	O
ATOM	4147	O	HOH	W	58	25.976	-1.070	65.387	1.00	24.91	O
ATOM	4150	O	HOH	W	59	33.452	-18.763	39.829	1.00	32.17	O
ATOM	4153	O	HOH	W	60	28.131	-20.142	36.740	1.00	36.39	O
ATOM	4156	O	HOH	W	61	10.277	-4.565	28.763	1.00	26.72	O
ATOM	4159	O	HOH	W	62	24.521	-10.754	55.710	1.00	22.10	O
ATOM	4162	O	HOH	W	63	30.024	3.202	61.463	1.00	25.62	O
ATOM	4165	O	HOH	W	64	8.046	-19.428	18.768	1.00	31.72	O
ATOM	4168	O	HOH	W	65	22.124	-15.298	25.264	1.00	23.76	O

Figure 5-45

ATOM	4171	O	HOH	W	66	9.340	-0.625	26.649	1.00	33.77
ATOM	4174	O	HOH	W	67	22.150	-20.929	47.436	1.00	22.53
ATOM	4177	O	HOH	W	68	10.935	-2.713	53.093	1.00	30.90
ATOM	4180	O	HOH	W	69	33.990	-11.990	18.450	1.00	32.26
ATOM	4183	O	HOH	W	70	29.560	-18.591	25.178	1.00	31.08
ATOM	4186	O	HOH	W	71	5.386	-9.782	29.237	1.00	25.46
ATOM	4189	O	HOH	W	72	30.818	-18.884	47.765	1.00	33.72
ATOM	4192	O	HOH	W	73	32.720	-19.019	31.299	1.00	33.74
ATOM	4195	O	HOH	W	74	11.308	-23.395	15.836	1.00	31.09
ATOM	4198	O	HOH	W	75	28.678	-2.741	22.843	1.00	27.62
ATOM	4201	O	HOH	W	76	40.782	-10.225	36.484	1.00	30.77
ATOM	4204	O	HOH	W	77	13.064	0.481	31.085	1.00	26.78
ATOM	4207	O	HOH	W	78	36.980	2.981	55.991	1.00	30.14
ATOM	4210	O	HOH	W	79	17.609	-6.759	50.465	1.00	31.64
ATOM	4213	O	HOH	W	80	6.075	-6.166	28.915	1.00	24.11
ATOM	4216	O	HOH	W	81	37.218	-17.210	45.282	1.00	28.55
ATOM	4219	O	HOH	W	82	31.430	13.439	44.059	1.00	30.71
ATOM	4222	O	HOH	W	83	11.061	-11.145	39.944	1.00	45.28
ATOM	4225	O	HOH	W	84	13.995	-3.709	27.604	1.00	30.24
ATOM	4228	O	HOH	W	85	-8.547	14.167	34.457	1.00	41.17
ATOM	4231	O	HOH	W	86	12.154	-1.563	29.674	1.00	29.34
ATOM	4234	O	HOH	W	87	40.567	0.285	31.901	1.00	39.11
ATOM	4237	O	HOH	W	88	18.416	-2.791	21.845	1.00	30.88
ATOM	4240	O	HOH	W	89	20.045	0.302	61.898	1.00	24.40
ATOM	4243	O	HOH	W	90	21.244	8.081	26.469	1.00	39.02
ATOM	4246	O	HOH	W	91	23.587	6.698	66.965	1.00	34.37
ATOM	4249	O	HOH	W	92	-3.668	12.465	40.745	1.00	39.57
ATOM	4252	O	HOH	W	93	36.621	2.042	28.430	1.00	35.94
ATOM	4255	O	HOH	W	94	40.898	-3.589	33.858	1.00	34.53
ATOM	4258	O	HOH	W	95	40.576	-14.574	47.625	1.00	36.03
ATOM	4261	O	HOH	W	96	0.613	9.514	30.164	1.00	36.36
ATOM	4264	O	HOH	W	97	11.628	-17.713	20.705	1.00	34.25
ATOM	4267	O	HOH	W	98	24.954	7.668	25.927	1.00	27.16
ATOM	4270	O	HOH	W	99	15.390	7.025	38.027	1.00	29.40
ATOM	4273	O	HOH	W	100	22.625	-6.941	49.347	1.00	39.05
ATOM	4276	O	HOH	W	101	8.373	-22.481	15.596	1.00	33.81
ATOM	4279	O	HOH	W	102	30.369	5.278	59.776	1.00	33.74
ATOM	4282	O	HOH	W	103	41.338	-2.707	37.675	1.00	29.29
ATOM	4285	O	HOH	W	104	28.791	-11.742	59.148	1.00	39.32
ATOM	4288	O	HOH	W	105	11.634	-26.143	18.788	1.00	36.81
ATOM	4291	O	HOH	W	106	7.819	-7.870	52.253	1.00	39.46
ATOM	4294	O	HOH	W	107	-1.143	11.518	42.825	1.00	38.53
ATOM	4297	O	HOH	W	108	31.520	-20.537	29.068	1.00	

[illegible]

Figure S-46

ATOM	4318	O	HOH W 115	25.866	-13.362	18.161	1.00	36.61	O
ATOM	4321	O	HOH W 116	13.281	4.205	52.743	1.00	42.27	O
ATOM	4324	O	HOH W 117	38.297	4.475	47.147	1.00	33.36	O
ATOM	4327	O	HOH W 118	-2.236	10.267	44.511	1.00	37.52	O
ATOM	4330	O	HOH W 119	37.565	5.895	49.683	1.00	46.73	O
ATOM	4333	O	HOH W 120	33.584	-5.835	22.780	1.00	32.49	O
ATOM	4336	O	HOH W 121	35.462	-21.282	38.394	1.00	55.47	O
ATOM	4339	O	HOH W 122	16.865	-19.547	21.306	1.00	27.44	O
ATOM	4342	O	HOH W 123	12.379	8.941	51.215	1.00	39.45	O
ATOM	4345	O	HOH W 124	7.524	-12.914	23.783	1.00	37.37	O
ATOM	4348	O	HOH W 125	7.002	7.918	39.410	1.00	39.86	O
ATOM	4351	O	HOH W 126	39.630	13.233	34.512	1.00	36.50	O
ATOM	4354	O	HOH W 127	35.097	-11.399	62.096	1.00	37.48	O
ATOM	4357	O	HOH W 128	21.607	3.999	24.843	1.00	41.76	O
ATOM	4360	O	HOH W 129	22.478	-15.210	21.158	1.00	33.88	O
ATOM	4363	O	HOH W 130	23.548	-6.336	46.901	1.00	27.09	O
ATOM	4366	O	HOH W 131	39.223	-3.552	31.628	1.00	34.54	O
ATOM	4369	O	HOH W 132	16.042	-7.439	27.693	1.00	35.28	O
ATOM	4372	O	HOH W 133	30.069	15.041	50.355	1.00	37.56	O
ATOM	4375	O	HOH W 134	-12.054	-1.413	27.623	1.00	46.27	O
ATOM	4378	O	HOH W 135	24.926	-21.915	31.263	1.00	35.51	O
ATOM	4381	O	HOH W 136	33.484	17.088	33.716	1.00	41.28	O
ATOM	4384	O	HOH W 137	37.571	-15.077	22.999	1.00	46.63	O
ATOM	4387	O	HOH W 138	-4.651	10.305	28.753	1.00	40.45	O
ATOM	4390	O	HOH W 139	7.244	3.278	47.459	1.00	37.56	O
ATOM	4393	O	HOH W 140	25.957	14.697	25.537	1.00	46.95	O
ATOM	4396	O	HOH W 141	19.573	8.296	56.060	1.00	52.38	O
ATOM	4399	O	HOH W 142	26.323	-21.066	39.242	1.00	42.83	O
ATOM	4402	O	HOH W 143	25.430	-19.884	49.691	1.00	43.36	O
ATOM	4405	O	HOH W 144	13.134	-30.765	15.684	1.00	45.93	O
ATOM	4408	O	HOH W 145	29.414	-21.756	28.642	1.00	50.58	O
ATOM	4411	O	HOH W 146	28.351	-18.821	51.770	1.00	41.18	O
ATOM	4414	O	HOH W 147	12.847	-23.572	13.257	1.00	46.60	O
ATOM	4417	O	HOH W 148	8.003	11.514	41.950	1.00	32.62	O
ATOM	4420	O	HOH W 149	38.748	-13.077	22.902	1.00	39.48	O
ATOM	4423	O	HOH W 150	8.343	10.168	38.934	1.00	42.90	O
ATOM	4426	O	HOH W 151	17.499	-5.735	26.996	1.00	29.41	O
ATOM	4429	O	HOH W 152	18.497	-0.355	36.152	1.00	26.83	O
ATOM	4432	O	HOH W 153	10.174	-26.483	16.855	1.00	37.80	O
ATOM	4435	O	HOH W 154	11.960	-1.336	55.400	1.00	43.14	O
ATOM	4438	O	HOH W 155	29.996	15.804	31.898	1.00	35.23	O
ATOM	4441	O	HOH W 156	28.284	-14.512	16.257	1.00	40.72	O
ATOM	4444	O	HOH W 157	41.746	5.776	38.906	1.00	36.43	O
ATOM	4447	O	HOH W 158	-10.695	2.291	31.483	1.00	42.36	O
ATOM	4450	O	HOH W 159	37.788	-19.823	39.112	1.00	47.59	O
ATOM	4453	O	HOH W 160	23.881	6.960	58.056	1.00	35.00	O
ATOM	4456	O	HOH W 161	37.835	-14.490	31.875	1.00	34.79	O
ATOM	4459	O	HOH W 162	35.191	5.005	55.163	1.00	40.96	O
ATOM	4462	O	HOH W 163	21.856	10.212	28.395	1.00	42.57	O
ATOM	4465	O	HOH W 164	-7.866	11.842	42.057	1.00	53.86	O
ATOM	4468	O	HOH W 165	35.283	-3.744	22.596	1.00	42.31	O
ATOM	4471	O	HOH W 166	29.408	17.784	33.686	1.00	51.95	O
ATOM	4474	O	HOH W 167	19.792	8.386	31.441	1.00	36.33	O
ATOM	4477	O	HOH W 168	39.386	-12.644	30.998	1.00	43.83	O
ATOM	4480	O	HOH W 169	14.210	8.710	34.935	1.00	38.49	O

ATOM	4483	O	HOH	W	170	-5.030	17.943	30.092	1.00	55.72	O
ATOM	4486	O	HOH	W	171	44.458	-4.818	59.172	1.00	43.22	O
ATOM	4489	O	HOH	W	172	-10.799	5.249	33.071	1.00	52.86	O
ATOM	4492	O	HOH	W	173	8.773	-12.249	21.595	1.00	42.84	O
ATOM	4495	O	HOH	W	174	39.315	13.813	31.995	1.00	40.45	O
ATOM	4498	O	HOH	W	175	19.345	-4.575	27.677	1.00	26.54	O
ATOM	4501	O	HOH	W	176	9.152	4.798	41.127	1.00	44.65	O
ATOM	4504	O	HOH	W	177	28.512	-22.950	39.300	1.00	56.07	O
ATOM	4507	O	HOH	W	178	41.587	-8.759	40.287	1.00	41.14	O
ATOM	4510	O	HOH	W	179	21.621	6.663	57.083	1.00	36.44	O
ATOM	4513	O	HOH	W	180	9.788	-6.595	52.966	1.00	39.02	O
ATOM	4516	O	HOH	W	181	32.993	5.439	58.873	1.00	37.18	O
ATOM	4519	O	HOH	W	182	-10.042	7.844	34.829	1.00	60.37	O
ATOM	4522	O	HOH	W	183	20.861	-6.982	62.399	1.00	32.09	O
ATOM	4525	O	HOH	W	184	-6.232	14.991	37.302	1.00	42.96	O
ATOM	4528	O	HOH	W	185	-7.879	13.524	37.344	1.00	56.51	O
ATOM	4531	O	HOH	W	186	35.635	-18.895	25.202	1.00	60.71	O
ATOM	4534	O	HOH	W	187	13.615	-5.237	56.777	1.00	48.24	O
ATOM	4537	O	HOH	W	188	32.787	13.021	46.944	1.00	42.47	O
ATOM	4540	O	HOH	W	189	17.043	10.116	36.657	1.00	50.03	O
ATOM	4543	O	HOH	W	190	41.663	10.689	42.712	1.00	40.86	O
ATOM	4546	O	HOH	W	191	-10.897	3.639	28.980	1.00	49.46	O
ATOM	4549	O	HOH	W	192	23.217	-25.005	43.748	1.00	41.96	O
ATOM	4552	O	HOH	W	193	0.389	5.266	38.980	1.00	40.10	O
ATOM	4555	O	HOH	W	194	24.283	-18.189	53.591	1.00	39.92	O
ATOM	4558	O	HOH	W	195	33.143	-19.554	25.314	1.00	45.80	O
ATOM	4561	O	HOH	W	196	42.547	2.043	37.753	1.00	36.29	O
ATOM	4564	O	HOH	W	197	26.096	-25.410	42.175	1.00	51.95	O
ATOM	4567	O	HOH	W	198	19.467	5.706	28.424	1.00	38.46	O
ATOM	4570	O	HOH	W	199	41.634	-3.401	46.403	1.00	37.73	O
ATOM	4573	O	HOH	W	200	8.916	-29.184	15.174	1.00	32.07	O
ATOM	4576	O	HOH	W	201	-5.981	13.741	39.552	1.00	43.85	O
ATOM	4579	O	HOH	W	202	20.014	6.137	59.702	1.00	49.66	O
ATOM	4582	O	HOH	W	203	34.515	-16.284	22.972	1.00	49.72	O
ATOM	4585	O	HOH	W	204	13.868	9.800	45.959	1.00	49.78	O
ATOM	4588	O	HOH	W	205	-9.716	5.553	30.224	1.00	51.40	O
ATOM	4591	O	HOH	W	206	-1.734	2.388	27.339	1.00	46.37	O
ATOM	4594	O	HOH	W	207	26.024	-26.041	39.793	1.00	68.04	O
ATOM	4597	O	HOH	W	208	12.610	1.249	53.646	1.00	46.84	O
ATOM	4600	O	HOH	W	209	10.206	1.865	27.799	1.00	48.09	O